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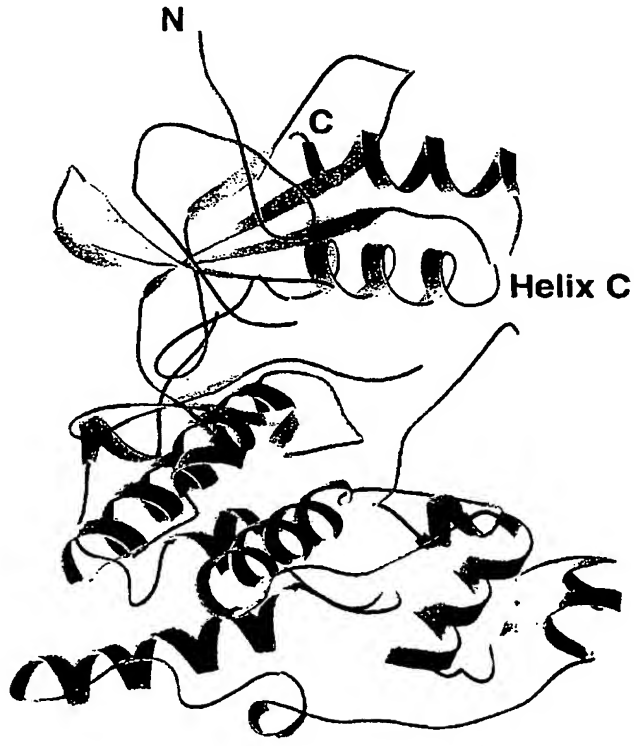
(54) Title: CRYSTAL STRUCTURES OF JNK-INHIBITOR COMPLEXES AND BINDING POCKETS THEREOF



(57) Abstract: The invention relates to crystalline molecules or molecular complexes that comprise binding pockets of c-Jun N-terminal kinase 3 (JNK3) or its homologues. The invention also relates to crystals comprising JNK3 and an inhibitor. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of JNK3 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the molecule or molecular complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compounds, including agonists and antagonists, which bind to JNK3 or homologues thereof.

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CRYSTAL STRUCTURES OF JNK-INHIBITOR COMPLEXES AND BINDING POCKETS THEREOF

TECHNICAL FIELD OF INVENTION

[0001] The present invention relates to crystalline molecules or molecular complexes that comprise binding pockets of the c-Jun N-terminal kinase 3 (JNK3) and its homologues, the structure of these molecules or molecular complexes, and methods of using these molecules or molecular complexes.

BACKGROUND OF THE INVENTION

[0002] Mammalian cells respond to extracellular stimuli by activating signaling cascades that are mediated by members of the mitogen-activated protein (MAP) kinase family, which include the extracellular signal regulated kinases (ERKs), the p38 MAP kinases and the c-Jun N-terminal kinases (JNK). MAP kinases are serine/threonine kinases that are activated by dual phosphorylation of threonine and tyrosine at the Thr-X-Tyr segment in the activation loop. MAP kinases phosphorylate various substrates including transcription factors, which in turn regulate the expression of specific sets of genes and thus mediate a specific response to a specific stimulus.

[0003] Three distinct genes, JNK1, JNK2, JNK3 have

been identified and at least ten different splicing isoforms of JNK exist in mammalian cells [S. Gupta et al., EMBO J., 15, pp. 2760-2770 (1996)]. Members of the JNK kinases are activated by proinflammatory cytokines tumor necrosis factor-alpha and interleukin-1 beta as well as environmental stress, such as anisomycin, UV irradiation, hypoxia, and osmotic shock [A. Minden et al., Biochemica et Biophysica Acta, 1333, F85-F104 (1997)]. The down-stream substrates of JNK proteins include transcription factors c-Jun, ATF-2, Elk1, p53 and a cell death domain protein (DENN) [Y. Zhang et al. Proc. Natl. Acad. Sci. USA, 95, pp. 2586-2591 (1998)]. Each of the JNK isoforms binds to these substrates with a different affinity, suggesting a regulation of signaling pathways by substrate specificity of different JNK proteins *in vivo* [S. Gupta et al., 1996].

[0004] JNK1 and JNK2 are widely expressed in a variety of tissues. In contrast, JNK3 is selectively expressed in the brain and to a lesser extent in the heart and testis [S. Gupta et al., (1996), *supra*; A. A. Mohit et al., Neuron, 14, pp. 67-78 (1995); J.H. Martin et al., Brain Res. Mol. Brain Res., 35, pp. 47-57 (1996)]. In the adult human brain, JNK3 expression is localized to a subpopulation of pyramidal neurons in the CA1, CA4 and subiculum regions of the hippocampus and layers 3 and 5 of the neocortex [A. A. Mohit et al. (1995), *supra*]. The CA1 neurons of patients with acute hypoxia showed strong nuclear JNK3-immunoreactivity compared to minimal, diffuse cytoplasmic staining of the hippocampal neurons from brain tissues of normal patients [Y. Zhang et al. (1998), *supra*]. In addition, JNK3 co-localizes immunochemically with neurons

vulnerable in Alzheimer's disease [A. A. Mohit et al., (1995), *supra*]. Disruption of the JNK3 gene caused resistance of mice to the excitotoxic glutamate receptor agonist kainic acid, which affected seizure activity, AP-1 transcriptional activity and apoptosis of hippocampal neurons, indicating that the JNK3 signaling pathway is a critical component in the pathogenesis of glutamate neurotoxicity (D. D. Yang et al., Nature, 389, pp. 865-870 (1997)]. Thus, selective modulation of JNK3 activity could potentially provide therapeutic intervention for neurodegenerative diseases such as stroke and epilepsy.

[0005] Accordingly, there has been an interest in identifying JNK3 inhibitors that are effective as therapeutic agents. A challenge has been to provide protein kinase inhibitors that act in a selective manner. Since there are numerous protein kinases that are involved in a variety of cellular responses, non-selective inhibitors may lead to unwanted side effects.

[0006] Further, the binding of different inhibitors may alter the conformation of the binding pocket. Information provided by the X-ray crystal structure of JNK3-inhibitor complexes would be extremely useful in iterative drug design of various JNK proteins. The determination of the amino acid residues in JNK3 binding pockets and the determination of the shape of those binding pockets would allow one to modify inhibitors to bind more favorably to this class of enzymes.

SUMMARY OF THE INVENTION

[0007] Applicants have solved these problems by providing a crystal comprising JNK3 or homologue thereof in complex with an inhibitor. Solving these crystal structures has allowed applicants to determine the shape of the inhibitor-binding pocket and amino acid residues in the pocket. The invention also provides a method for crystallizing JNK-inhibitor complexes.

[0008] Thus, the present invention provides crystalline molecules or molecular complexes comprising the JNK3 inhibitor-binding pockets, or JNK3-like inhibitor-binding pockets that have similar three-dimensional shapes.

[0009] The invention further provides a computer comprising a data storage medium that comprises the structure coordinates of molecules and molecular complexes comprising all or part of the JNK3 or JNK3-like binding pockets and means for generating three-dimensional structural information from the structure coordinates. The computer may be used to produce three-dimensional information of the crystalline molecule or molecular complex comprising such binding pockets.

[0010] The invention provides methods for screening, designing, optimizing, evaluating and identifying compounds that bind to the molecules or molecular complexes or their binding pockets. The methods can be used to identify agonists and antagonists of JNK3 and its homologues.

[0011] The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which

contain at least some structurally similar features to JNK3, particularly JNK3 homologues. This is achieved by using at least some of the structural coordinates obtained from the JNK3-inhibitor structures.

BRIEF DESCRIPTION OF THE FIGURES

[0012] Figure 1 lists the atomic structure coordinates for unphosphorylated JNK3 in complex with N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide [see WO 200112621, incorporated herein by reference] (hereinafter "isoxazole1"), as derived by X-ray diffraction from a crystal of that complex.

[0013] Figure 2 lists the atomic structure coordinates for unphosphorylated JNK3 in complex with 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid phenylamide [see WO 2000075118, incorporated herein by reference] (hereinafter "uracil1") as derived by X-ray diffraction from a crystal of that complex.

[0014] Figure 3 lists the atomic structure coordinates for unphosphorylated JNK3 in complex with 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide] [see U.S. patent 6,274,738, incorporated herein by reference] (herein after "thiazole1") as derived by X-ray diffraction from a crystal of that complex.

[0015] The following abbreviations are used in Figure 1, 2 and 3:

[0016] "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

[0017] "Res" refers to the amino acid residue in the molecular model.

[0018] "X, Y, Z" define the atomic position of the element measured.

[0019] "B" is a thermal factor that measures movement of the atom around its atomic center.

[0020] "Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

[0021] Figure 4 is a structure-based sequence alignment of JNK3, ERK2, p38 and cAPK (SEQ ID NO: 1, 2, 3 and 4, respectively).

[0022] Figure 5 is a ribbon representation of the overall fold of JNK3. The N-terminal β strands and C-terminal α helices are shown.

[0023] Figure 6 shows a detailed comparison of the active site of JNK3-uracil1 with that of JNK3-AMP-PNP. The Cα of residues 140-149 of the two structures were superimposed. The figure illustrates the protein conformational changes induced by inhibitor binding. Figure 6A is viewed from the entrance of the cleft where ATP binds; Figure 6B is viewed perpendicular to 6A. Certain distances between atoms are indicated by dashed lines.

[0024] Figure 7 depicts an overlay of the structures of AMP-PNP, uracil1, thiazole1 and isoxazole1.

[0025] Figure 8 shows the three inhibitors bound in the inhibitor-binding pocket. Figure 8A (thiazole1), Figure 8B (uracil1), Figure 8C (isoxazole1). Hydrogen bonds are indicated by dashed lines.

[0026] Figure 9 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 10 and 11.

[0027] Figure 10 shows a cross section of a magnetic storage medium.

[0028] Figure 11 shows a cross section of a optically-readable data storage medium.

DETAILED DESCRIPTION OF THE INVENTION

[0029] In order that the invention described herein may be more fully understood, the following detailed description is set forth.

[0030] Throughout the specification, the word "comprise", or variations such as "comprises" or "comprising" will be understood to imply the inclusion of a stated integer or groups of integers but not exclusion of any other integer or groups of integers.

[0031] The following abbreviations are used throughout the application:

A =	Ala =	Alanine	T =	Thr =	Threonine
V =	Val =	Valine	C =	Cys =	Cysteine
L =	Leu =	Leucine	Y =	Tyr =	Tyrosine
I =	Ile =	Isoleucine	N =	Asn =	Asparagine
P =	Pro =	Proline	Q =	Gln =	Glutamine
F =	Phe =	Phenylalanine	D =	Asp =	Aspartic Acid
W =	Trp =	Tryptophan	E =	Glu =	Glutamic Acid
M =	Met =	Methionine	K =	Lys =	Lysine
G =	Gly =	Glycine	R =	Arg =	Arginine
S =	Ser =	Serine	H =	His =	Histidine

[0032] The term "about" when used in the context of RMSD values takes into consideration the standard error of the RMSD value, which is ± 0.1 Å.

[0033] The term "active site" refers to the portion of the protein kinase to which the nucleotide substrate binds. This site is located at the interface of the N-terminal α-helical and C-terminal β-strand domain, and is bordered by the glycine rich loop and the hinge [See, Xie et al., Structure, 6, pp. 983-991 (1998), incorporated herein by reference].

[0034] The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

[0035] The term "binding pocket" refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound.

[0036] The term "chemical entity" refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. The chemical entity may be, for example, a ligand, a substrate, a nucleotide triphosphate, a nucleotide diphosphate, phosphate, a nucleotide, an agonist, antagonist, inhibitor, antibody, drug, peptide, protein or compound.

[0037] The term "conservative substitutions" refers to residues that are physically or functionally similar to the corresponding reference residues. That is, a conservative substitution and its reference residue

have similar size, shape, electric charge, chemical properties including the ability to form covalent or hydrogen bonds, or the like. Preferred conservative substitutions are those fulfilling the criteria defined for an accepted point mutation in Dayhoff *et al.*, Atlas of Protein Sequence and Structure, 5, pp. 345-352 (1978 & Supp.), which is incorporated herein by reference. Examples of conservative substitutions are substitutions including but not limited to the following groups: (a) valine, glycine; (b) glycine, alanine; (c) valine, isoleucine, leucine; (d) aspartic acid, glutamic acid; (e) asparagine, glutamine; (f) serine, threonine; (g) lysine, arginine, methionine; and (h) phenylalanine, tyrosine.

[0038] The term "corresponding amino acid" or "residue which corresponds to" refers to a particular amino acid or analogue thereof in a JNK3 protein or JNK3 homologue that corresponds to an amino acid in JNK3α1. The corresponding amino acid is identical or functionally equivalent to the JNK3α1 amino acid to which it corresponds.

[0039] Methods for identifying a corresponding amino acid are known in the art and are based upon sequence, structural alignment, its functional position or a combination thereof as compared to the JNK3 kinase. For example, corresponding amino acids may be identified by superimposing the backbone atoms of the amino acids in JNK3 and the JNK3 homologue using well known software applications, such as QUANTA (Accelrys, San Diego, CA ©2001, 2002). The corresponding amino acids may also be identified using sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local

homology algorithm described by Smith and Waterman in Advances in Applied Mathematics 2, 482 (1981), which is incorporated herein by reference.

[0040] The term "crystallization solution" refers to a solution that promotes crystallization. The solution comprises at least one agent, and may include a buffer, one or more salts, a precipitating agent, one or more detergents, sugars or organic compounds, lanthanide ions, a poly-ionic compound and/or a stabilizer.

[0041] The term "domain" refers to a structural unit of the JNK3 protein or homologue. The domain can comprise a binding pocket, or a sequence or structural motif. In JNK3, the protein is separated into two domains, the N-terminal domain which contains β strands and the C-terminal domain which is predominantly α helical.

[0042] The term "generating a three-dimensional structure" refers to converting the lists of structure coordinates into structural models in three-dimensional space. This can be achieved through commercially or publicly available software. The three-dimensional structure may be displayed as a graphical representation or used to perform computer modeling or fitting operations. In addition, the structure coordinates themselves may be used to perform computer modeling and fitting operations.

[0043] The term "homology model" refers to a structural model derived from known three-dimensional structure(s). Generation of the homology model, termed "homology modeling", can include sequence alignment, residue replacement, residue conformation adjustment through energy minimization, or a combination thereof

[0044] The term "homologue of JNK3" or "JNK3 homologue" refers to a molecule that is homologous to JNK3 by three-dimensional structure or sequence and retains the kinase activity of a JNK protein. Examples of homologues include but are not limited to the following: JNK protein such as JNK1, JNK2 and JNK3 with conservative substitutions, additions, deletions or a combination thereof; other JNK proteins such as JNK1, JNK2 or isoforms thereof.

[0045] The term "JNK" refers to the kinases from the c-Jun N-terminal kinase family. Examples of this family of kinases include but are not limited to JNK1, JNK2, JNK3 and isoforms thereof. Isoforms of JNK1, JNK2 and JNK3 include but are not limited to JNK1α1, JNK1α2, JNK1β1, JNK1β2, JNK2α1, JNK2α2, JNK2β1, JNK2β2, JNK3α1, JNK3α2, JNK3β1, JNK3β2, respectively.

[0046] The term "JNK3 inhibitor-binding pocket" refers to that portion of the JNK3 enzyme active site to which the inhibitor binds. The inhibitor-binding pocket is defined by the structure coordinates of a certain set of amino acid residues present in the JNK3-inhibitor structure, as described below. The amino acid residues and the shape of the inhibitor-binding pocket according to this invention differ from those of the active site binding pocket described in the JNK3-AMP-PNP structure [WO 9957253].

[0047] The term "JNK3-like" refers to all or a portion of a molecule or molecular complex that has a commonality of shape to all or a portion of the JNK3 protein. In the JNK3-like inhibitor-binding pocket, the commonality of shape is defined by a root mean square deviation of the structure coordinates of the backbone atoms between the amino acids in the JNK3-like

inhibitor-binding pocket and the amino acids in the JNK3 inhibitor-binding pocket (as set forth in Figure 1 2 or 3).

[0048] The term "part of a JNK3 inhibitor-binding pocket" or "part of a JNK3-like inhibitor-binding pocket" refers to less than all of the amino acid residues that define the JNK3 or JNK3-like inhibitor-binding pocket. The structure coordinates of residues that constitute part of a JNK3 or JNK3-like inhibitor-binding pocket may be specific for defining the chemical environment of the binding pocket, or useful in designing fragments of an inhibitor that may interact with those residues. For example, the portion of residues may be key residues that play a role in ligand binding, or may be residues that are spatially related and define a three-dimensional compartment of the binding pocket. The residues may be contiguous or non-contiguous in primary sequence.

[0049] In one embodiment, part of the JNK3 or JNK3-like inhibitor-binding pocket is at least two amino acid residues. Preferably, the amino acids are Lys93 and Met146. In one embodiment, part of an inhibitor-binding pocket, comprises at least one residue that is not found within 5 or 8 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. Examples of these residues include Pro69, Met115, Leu126, Leu127, Asn128, Tyr143, Leu144, Val145, Lys198 and Ile205. In another embodiment, part of an inhibitor-binding pocket comprises at least one residue that underwent conformational change when compared to the residues in the JNK3-AMP-PNP structure. Examples of these residues include but are not limited to Lys93, Ile124, Leu126, Leu144 and Met146. In another embodiment, part of an

inhibitor-binding pocket comprises Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155. In another embodiment, part of any inhibitor-binding pocket comprises Ser72, Ser193 and Asn152.

[0050] The term "part of a JNK3 protein" or "part of a JNK3 homologue" refers to less than all of the amino acid residues of a JNK3 protein or homologue. In one embodiment, part of a JNK3 protein or homologue defines the binding pockets, domains or motifs of the protein or homologue. The structure coordinates of residues that constitute part of a JNK3 protein or homologue may be specific for defining the chemical environment of the protein, or useful in designing fragments of an inhibitor that may interact with those residues. The portion of residues may also be residues that are spatially related and define a three-dimensional compartment of a binding pocket, motif or domain. The residues may be contiguous or non-contiguous in primary sequence. For example, the portion of residues may be key residues that play a role in ligand or substrate binding, catalysis or structural stabilization.

[0051] The term "protein complex" refers to a protein associated with a chemical entity, for example, a ligand, a substrate, nucleotide triphosphate, an agonist, an antagonist, inhibitor, drug or compound. In one embodiment, the chemical entity is an inhibitor that induces the Met146 in JNK3 or corresponding methionine in a JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180° upon binding. In one embodiment, the chemical entity is selected from the group consisting of N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide, 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-

carboxylic acid phenylamide, 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide, 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol and 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide.

[0052] The term "motif" refers to a portion of the JNK3 kinase or homologue that defines a structural compartment or carries out a function in the protein, for example, catalysis, structural stabilization or phosphorylation. The motif may be conserved in sequence, structure and function when compared to other kinases or related proteins. The motif can be contiguous in primary sequence or three-dimensional space. The motif may comprise α-helices and β-sheets. Examples of a motif include but are not limited to a binding pocket, active site, phosphorylation lip or activation loop, the glycine-rich phosphate anchor loop, the catalytic loop and the DFG loop [See, Xie et al., Structure, 6, pp. 983-991 (1998)].

[0053] The term "root mean square deviation" or "RMSD" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. The "root mean square deviation" may define the variation in the backbone and/or sidechains of a protein from the backbone and/or sidechains of JNK3, a binding pocket, a motif, a domain, or portion thereof, as defined by the structure coordinates of JNK3 described herein.

[0054] The term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound to be diffused into the crystal.

[0055] The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein or protein complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the molecule or molecular complex.

[0056] The term "sufficiently homologous to JNK3" refers to a protein that has a sequence homology of at least 20% compared to JNK3 protein. In other embodiments, the sequence homology is at least 40%, at least 60%, at least 80%, at least 90% or at least 95%.

[0057] The term "three-dimensional structural information" refers to information obtained from the structure coordinates. Structural information generated can include the three-dimensional structure or graphical representation of the structure. Structural information can also be generated when subtracting distances between atoms in the structure coordinates, calculating chemical energies for a JNK3 molecule or molecular complex or homologues thereof, calculating or minimizing energies for an association of a JNK3 molecule or molecular complex or homologues thereof to a chemical entity.

Crystallizable Compositions and Crystals of JNK3-inhibitor Complexes

[0058] According to one embodiment, the invention provides a crystallizable composition or crystal comprising a JNK3 protein complexed with an inhibitor

or JNK3 homologue complexed with an inhibitor. In one embodiment, the JNK3 protein or homologue is phosphorylated or unphosphorylated. In another embodiment, the JNK3 protein is JNK3α1. In one embodiment, the inhibitor is capable of inducing the Met146 in JNK3 or corresponding methionine in a JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180° upon binding. In one embodiment, the inhibitor is selected from the group consisting of N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide, 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid phenylamide, 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide, 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol and 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide.

[0059] For JNK3 protein or a JNK3 protein with amino acid substitutions, the N-terminus of the protein can be truncated. Specifically, the JNK3 proteins contain an N-terminal extension of about 40 amino acids as compared to JNK1 and JNK2 proteins (see for example, GenBank entries for JNK1, JNK2 and JNK3 proteins, NP620637, S71102 and S71104, respectively). In one embodiment, those 40 amino acids are removed from JNK3 proteins in the crystallizable or crystal compositions of this invention.

[0060] In addition, any JNK3 protein or homologue thereof in these crystal or crystallizable compositions preferably has a C-terminal truncation of about 20 amino acids. The C-terminal truncation is helpful in obtaining diffraction quality crystals.

[0061] The crystallizable compositions may further comprise a crystallization solution of polyethylene

glycol monomethyl ether at between about 10 to 30% v/v, ethylene glycol at between about 5 to 20% v/v, a reducing agent, such as ß-mercaptoethanol at between about 5 to 50 mM, and a buffer that maintains pH at between about 7.0 and 7.5. Preferably, the buffer is 100 mM Hepes at pH 7.0.

[0062] In one embodiment, the crystal has a unit cell dimension of a= 54.75 Å b= 70.48 Å, c= 107.66 Å, $\alpha = \beta = \gamma = 90°$ and belongs to space group *P212121*. In another embodiment, the crystal has a unit cell dimension of a= 51.65 Å b= 71.01 Å, c= 106.7 Å, $\alpha = \beta = \gamma = 90°$ and belongs to space group *P212121*. In another embodiment, the crystal has a unit cell dimension of a= 50.74 Å b= 71.82 Å, c= 107.22 Å, $\alpha = \beta = \gamma = 90°$ and belongs to space group *P212121*. It will be readily apparent to those skilled in the art that the unit cells of the crystal compositions may deviate upto ± 1-2 Å from the above cell dimensions depending on the deviation in the unit cell calculations or conformational change in the protein.

[0063] The JNK3 protein or homologue thereof may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products. In one embodiment, the protein is overexpressed from an *E. coli* system.

[0064] The invention also relates to a method of making crystals of JNK3-inhibitor complexes or JNK3 homologue-inhibitor complexes. Such methods comprise the steps of:

a) producing a composition comprising a crystallization solution and a JNK3 protein or homologue thereof complexed with an inhibitor; and

b) subjecting said composition to devices or conditions which promote crystallization.

[0065] In one embodiment, the inhibitor is capable of inducing the Met146 in JNK3 or corresponding methionine in the JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180° upon binding. In another embodiment, the inhibitor is selected from the group consisting of N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide, 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid phenylamide, 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide, 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol and 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide. In another embodiment, the crystallization solution is as described previously. In another embodiment, the composition is treated with micro-crystals of JNK3 or JNK3 complexes or homologues thereof after step (a) but prior to step (b).

[0066] In each of the above embodiments, it is preferred that the JNK3 protein is JNK3α1.

[0067] Devices for promoting crystallization can include but are not limited to the hanging-drop, sitting-drop, dialysis or microtube batch devices. [U.S. patent 4,886,646, 5,096,676, 5,130,105, 5,221,410 and 5,400,741; Pav *et al.*, Proteins: Structure, Function, and Genetics, 20, pp. 98-102 (1994), incorporated herein by reference]. The hanging-drop or sitting-drop methods produce crystals by vapor

diffusion. The hanging-drop, sitting-drop, and some adaptations of the microbatch methods [D'Arcy et al., J. Cryst. Growth, 168, pp. 175-180 (1996) and Chayen, J. Appl. Cryst., 30, pp. 198-202 (1997)] produce crystals by vapor diffusion. The hanging drop and sitting drop containing the crystallizable composition is equilibrated in a reservoir containing a higher or lower concentration of the precipitant. As the drop approaches equilibrium with the reservoir, the saturation of protein in the solution leads to the formation of crystals.

[0068] Microseeding or seeding may be used to obtain larger, or better quality (i.e., crystals with higher resolution diffraction or single crystals) crystals from initial micro-crystals. Microseeding involves the use of crystalline particles to provide nucleation under controlled crystallization conditions. Microseeding is used to increase the size and quality of crystals. In this instance, micro-crystals are crushed to yield a stock seed solution. The stock seed solution is diluted in series. Using a needle, glass rod or strand of hair, a small sample from each diluted solution is added to a set of equilibrated drops containing a protein concentration equal to or less than a concentration needed to create crystals without the presence of seeds. The aim is to end up with a single seed crystal that will act to nucleate crystal growth in the drop.

[0069] It would be readily apparent to one of skill in the art following the teachings of the specification to vary the crystallization conditions disclosed herein to identify other crystallization conditions that would produce crystals of JNK3 homologue, JNK3 homologue

complex, other JNK3 proteins or JNK3 protein complexes. Such variations include, but are not limited to, adjusting pH, protein concentration and/or crystallization temperature, changing the identity or concentration of salt and/or precipitant used, using a different method of crystallization, or introducing additives such as detergents (e.g., TWEEN 20 (monolaurate), LDAO, Brij 30 (4 lauryl ether)), sugars (e.g., glucose, maltose), organic compounds (e.g., dioxane, dimethylformamide), lanthanide ions or polyionic compounds that aid in crystallization. High throughput crystallization assays may also be used to assist in finding or optimizing the crystallization conditions.

Binding Pockets of JNK3 Protein or Homologues thereof

[0070] As mentioned above, applicants have solved the three-dimensional X-ray crystal structure of JNK3α1 in complex with inhibitors. The atomic coordinate data is presented in Figures 1, 2 and 3.

[0071] In order to use the structure coordinates generated for the JNK3-inhibitor complex or one of its binding pockets or homologues thereof, it is often times necessary to convert the structure coordinates into a three-dimensional shape. This is achieved through the use of commercially available software that is capable of generating the three-dimensional structure of molecules or portions thereof from a set of structure coordinates.

[0072] Binding pockets, also referred to as binding sites in the present invention, are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the

binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential inhibitors of the binding sites of biologically important targets.

[0073] The structure coordinates described above may be used to derive the torsion angles of the side chains [S.C. Lovell et al, Proteins: Structure, Function, and Genetics, 40, 389-408, (2000)]. For example, in methionine, $\chi 1$ defines the torsion angle between N, Cα, Cβ, Sγ; $\chi 2$ defines the torsion angle between Cα, Cβ, Sγ, Cδ; and $\chi 3$ defines the torsion angle between Cβ, Sγ, Cδ, Cϵ.

[0074] Surprisingly, it has now been found that for the JNK3-isoxazole1 and JNK3-uracil1 complexes (Figure 1 and 2), the conformation of Met146 is very different from the conformations reported for methionines at this position in JNK3-AMP-PNP and other protein kinases. A novel hydrophobic pocket is formed around Met146 upon binding of isoxazole1 and uracil1. In order to compare the conformations of JNK3 and other protein kinases at a particular amino acid site, such as Met146, along the polypeptide backbone, well-known procedures may be used for performing sequence alignments of the amino acids. Such sequence alignments allow for the equivalent sites to be compared (see Figure 4). One such method for

performing a sequence alignment is the "bestfit" program available from Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in Advances in Applied Mathematics 2, 482 (1981).

[0075] A suitable amino acid sequence alignment will require that the proteins being aligned share a minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids. Hanks et al., Science, 241, 42 (1988); Hanks and Quinn, Methods in Enzymology, 200, 38 (1991).

[0076] Equivalents of the Met146 residue of JNK3 may also be identified by its functional position. Met146 is located in the beginning of the hinge region, and is adjacent to residue Glu147. Glu147 uses its backbone carbonyl to form a hydrogen bond with the amino group (N6) of the adenine base from AMP-PNP in the JNK3-AMP-PNP structure [Xie et al., Structure, 6, pp. 983-991 (1998)]. A comparison of the torsion angles between Met146 in the JNK3-inhibitor complexes and those of corresponding methionines in other kinases are illustrated in Table 1. The torsion angles were determined by the program QUANTA.

Table 1

Proteins	$\chi 1$ (°)	$\chi 2$ (°)	$\chi 3$ (°)
JNK3-isoxazole1	-159	-162	106
JNK3-uracil1	72	165	-55
JNK3-thiazole1	-54	128	-59
JNK3-AMP-PNP	-35	154	-86
P38γ-AMP-PNP [a] (Met109)	-55	107	56
JNK3-compound1 [b]	-173	-164	125
JNK3-compound2 [c]	144	-127	-164

a Bellon et al., Structure Fold Des., 7, pp.1057 (1999); PDB accession number 1CM8.

b Compound1 is 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol [see United States Patent 5,916,891, incorporated herein by reference.]

c Compound2 is 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide [see United States Patent 6,147,080, incorporated herein by reference].

[0077] In addition, applicants have determined that JNK3 amino acids Ile70, Ser72, Val78, Ala91, Ile92, Lys93, Ile124, Leu126, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Ser193, Val196 and Leu206 are within 5 Å of isoxazole1. These amino acids were identified using the program CNX (Accelrys, ©2001). Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in Figure 1 is considered a JNK3-inhibitor

binding pocket of this invention. These amino acids differ from the amino acids that are within 5 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. For example, in the JNK3-AMP-PNP structure, Leu126, Leu144 and Val145 were not found to be within 5 Å of the AMP-PNP.

[0078] Applicants have determined that in addition to the above amino acids, JNK3 amino acids Pro69, Gly71, Gln75, Gly76, Ile77, Cys79, Ala80, Val90, Lys94, Leu95, Met115, Ser125, Leu127, Asn128, Tyr143, Leu153, Gln155, Pro192, Asn194, Ile195, Val197, Lys204 and Asp207 are within 8 Å of isoxazole1. These amino acids were identified using the program CNX (Accelrys, ©2001) Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in Figure 1 is considered a JNK3-inhibitor binding pocket of this invention. These amino acids differ from the amino acids that are within 8 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. For example, in the JNK3-AMP-PNP structure, Pro69, Met115, Leu126, Leu127, Asn128, Tyr143 were not found to be within 8 Å of the AMP-PNP.

[0079] Applicants have also determined that JNK3 amino acids Ile70, Gln75, Val78, Ala91, Ile92, Lys93, Ile124, Leu126, Leu144, Val145, Met146, Leu148, Met149, Asp150, Ala151, Asn152, Ser193, Asn194, Val196 and Leu206 are within 5 Å of uracil1. These amino acids were identified using the program CNX (Accelrys, ©2001). Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in Figure 2 is considered a JNK3-inhibitor binding pocket of this invention. These amino acids differ from the amino acids that are within 5 Å of the

AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. For example, in the JNK3-AMP-PNP structure, Leu126, Leu144 and Val145 were not found to be within 5 Å of the AMP-PNP.

[0080] Applicants have determined that in addition to the above amino acids, JNK3 amino acids Gly73, Gly76, Ile77, Cys79, Ala80, Val90, Lys94, Leu95, Arg107, Glu111, Met115, Ser125, Leu127, Asn128, Tyr143, Glu147, Leu153, Cys154, Gln155, Pro192, Ile195, Val197, Ile205 and Asp207 are within 8 Å of uracil1. These amino acids were identified using the program CNX (Accelrys, ©2001). Thus, a binding pocket defined by the structural coordinates of these amino acids, as set forth in Figure 2 is considered a JNK3-inhibitor binding pocket of this invention. These amino acids differ from the amino acids that are within 8 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. For example, in the JNK3-AMP-PNP structure, Met115, Leu126, Leu127, Asn128, Tyr143, Ile205 were not found to be within 8 Å of the AMP-PNP.

[0081] In the above inhibitor-binding pockets (Figure 1 or 2), Leu144, Met146, Ile124, Leu126 and Lys93 show significant variation in conformation from those residues in the JNK3-AMP-PNP structure [WO 9957253].

[0082] Applicants have also determined that JNK3 amino acids Ile70, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Val196 and Leu206 are within 5 Å of thiazole1. These amino acids were identified using the program CNX (Accelrys, ©2001). Thus, a binding pocket defined by the structural coordinates of those amino acids, as set forth in Figure 3 is considered a JNK3-inhibitor

binding pocket of this invention. Compared to these amino acids, there are more amino acids that are within 5 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253].

[0083] Applicants have determined that in addition to the above amino acids, JNK3 amino acids Gly71, Ser72, Ile77, Cys79, Ala80, Val90, Ile92, Lys94, Leu95, Met115, Ser125, Leu144, Val145, Leu153, Cys154, Ser193, Asn194, Ile195, Val197, Lys198, Lys204, Ile205 and Asp207 are within 8 Å of thiazole1. These amino acids were identified using the program CNX (Accelrys, ©2001). Thus, a binding pocket defined by the structural coordinates of those amino acids, as set forth in Figure 3 is considered a JNK3-inhibitor binding pocket of this invention. These amino acids differ from the amino acids that are within 8 Å of the AMP-PNP in the JNK3-AMP-PNP structure [WO 9957253]. For example, in the JNK3-AMP-PNP structure, Met115, Lys198, Ile205 were not found to be within 8 Å of the AMP-PNP.

[0084] In addition, applicants have identified an inhibitor-binding pocket in the JNK3-thiazole1 structure that regulates the binding affinity of inhibitors. This inhibitor-binding pocket is defined by JNK3 amino acids Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155 according to Figure 3.

[0085] Applicants have also identified an inhibitor-binding pocket in the JNK3-uracil1 structure that may regulate the binding affinity of inhibitors. This inhibitor-binding pocket is defined by JNK3 amino acids Ser72, Ser193 and Asn152.

[0086] It will be readily apparent to those of skill in the art that the numbering of amino acids in other

isoforms of JNK3 or JNK3 homologues may be different than that set forth for JNK3α1. Corresponding amino acids in other isoforms of JNK3 or JNK3 homologues are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs.

[0087] Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

[0088] The variations in coordinates discussed above may be generated because of mathematical manipulations of the JNK3-inhibitor structure coordinates. For example, the structure coordinates set forth in Figure 1, 2 or 3 may undergo crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

[0089] Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal may also account for variations in structure coordinates. If such variations are within an acceptable standard error

as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same. Thus, for example, a ligand that bound to the inhibitor-binding pocket of JNK3 would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the RMSD value.

[0090] Various computational analyses may be necessary to determine whether a binding pocket, motif, domain or portion thereof of a molecule or molecular complex is sufficiently similar to the binding pocket, motif, domain or portion thereof of JNK3. Such analyses may be carried out in well known software applications, such as ProFit [A. C.R. Martin, ProFit version 1.8, http://www.bioinf.org.uk/software], Swiss-Pdb Viewer [Guex et al., Electrophoresis, 18, pp. 2714-2723 (1997)], the Molecular Similarity application of QUANTA [Accelrys, San Diego, CA © 2001, 2002] and as described in the accompanying User's Guide, which are incorporated herein by reference.

[0091] The above programs permit comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in QUANTA and Swiss-Pdb Viewer to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation on the structures; and 4) analyze the results. The procedure used in ProFit to compare structures includes the following steps: 1) load the structures to be compared; 2) specify selected residues of interest; 3) define the atom equivalences in the selected residues; 4) perform a

fitting operation on the selected residues; and
5) analyze the results.

[0092] Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA is defined by user input, protein backbone atoms (N, Cα, C and O) or all protein atoms may be defined as equivalent atoms for JNK3 amino acids and corresponding amino acids in the structures being compared.

[0093] The corresponding amino acids may be identified by sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in Advances in Applied Mathematics 2, 482 (1981), which is incorporated herein by reference. A suitable amino acid sequence alignment will require that the proteins being aligned share minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids [Hanks et al., Science, 241, 42 (1988); Hanks and Quinn, Methods in Enzymology, 200, 38 (1991)]. The identification of equivalent residues can also be assisted by secondary structure alignment, for example, aligning the α-helices, β-sheets in the structure. The program Swiss-Pdb viewer utilizes a best fit algorithm that is based on secondary sequence alignment.

[0094] When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting

operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

[0095] The RMSD values between the backbone atoms of amino acid residues in the inhibitor-binding pocket of JNK3-inhibitor complexes (Figure 1 or 2) and those of the corresponding amino acid residues in the JNK3-AMP-PNP complex are illustrated in Table 2. Amino acid residues Lys93, Ile124, Leu126, Leu144, Met146 (SET1) and amino acid residues Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155 (SET2) in the JNK3 inhibitor-binding pocket were used in the RMSD calculation. In addition, the RMSD values of the backbone atoms of the amino acid residues of JNK3-isoxazole1, JNK3-uracil1 and JNK3-thiazole1 compared to those of JNK3-AMP-PNP is 0.99 Å, 0.77 Å and 0.56 Å, respectively. The RMSD values of all atoms (including backbone and sidechain atoms) of the amino acid residues of JNK3-isoxazole1, JNK3-uracil1 and JNK3-thiazole1 compared to those of JNK3-AMP-PNP is 1.41 Å, 0.97 Å and 0.90 Å, respectively. The RMSD values are averages of individual RMSD values and were calculated by the program QUANTA.

Table 2

Proteins	RMSD of SET1 amino acids (Å)	RMSD of SET2 amino acids (Å)
JNK3-isoxazole1 and JNK3-AMP-PNP [a]	0.43	
JNK3-uracil1 and JNK3-AMP-PNP	0.37	1.15

a Xie et al., Structure, 6, pp. 983-991 (1998); PDB accession number 1JNK. The Protein Data Bank is an international repository for three dimensional structures and can be located at www.rcsb.org/pdb/.

[0096] For the purpose of this invention, any molecule, molecular complex, binding pocket, motif, domain thereof or portion thereof that is within a root mean square deviation for backbone atoms (N, Cα, C, O) when superimposed on the relevant backbone atoms described by structure coordinates listed in Figure 1, 2 or 3 are encompassed by this invention.

[0097] Therefore, one embodiment of this invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Ser72, Val78, Ala91, Ile92, Lys93, Ile124, Leu126, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Ser193, Val196 and Leu206 according to Figure 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues

of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.5, 0.3 or 0.2 Å.

[0098] The above set of amino acid residues may further comprise amino acid residues which correspond to JNK3 amino acid residues Pro69, Gly71, Gln75, Gly76, Ile77, Cys79, Ala80, Val90, Lys94, Leu95, Met115, Ser125, Leu127, Asn128, Tyr143, Leu153, Gln155, Pro192, Asn194, Ile195, Val197, Lys204 and Asp207 according to Figure 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.8, 0.6, 0.4 or 0.2 Å.

[0099] One embodiment of this invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Gln75, Val78, Ala91, Ile92, Lys93, Ile124, Leu126, Leu144, Val145, Met146, Leu148, Met149, Asp150, Ala151, Asn152, Ser193, Asn194, Val196 and Leu206 according to Figure 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.6, 0.4 or 0.2 Å.

[0100] The above set of amino acid residues may further comprise amino acid residues which correspond to JNK3 amino acid residues Gly73, Gly76, Ile77, Cys79, Ala80, Val90, Lys94, Leu95, Arg107, Glu111, Met115, Ser125, Leu127, Asn128, Tyr143, Glu147, Leu153, Cys154, Gln155, Pro192, Ile195, Val197, Ile205 and Asp207 according to Figure 2, wherein the root mean square

deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.7, 0.5, 0.3 or 0.2 Å.

[0101] One embodiment of this invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Val196 and Leu206 according to Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.4, 0.3 or 0.2 Å.

[0102] The above set of amino acid residues may further comprise JNK3 amino acid residues Gly71, Ser72, Ile77, Cys79, Ala80, Val90, Ile92, Lys94, Leu95, Met115, Ser125, Leu144, Val145, Leu153, Cys154, Ser193, Asn194, Ile195, Val197, Lys198, Lys204, Ile205 and Asp207 according to Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.5, 0.3 or 0.2 Å.

[0103] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Lys93 and Met146 according to Figure 1 or 2, wherein the root mean square deviation of the backbone atoms between said set

of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.2 Å.

[0104] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Lys93, Ile124, Leu126, Leu144 and Met146 according to Figure 1 or 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.3 Å or 0.2 Å.

[0105] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ser193 and Asn152 according to Figure 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.2 Å.

[0106] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155 according to Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid

residues is not greater than about 1.0, 0.8, 0.6, 0.4 or 0.2 Å.

[0107] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues set forth in Figure 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.9, 0.7, 0.5 or 0.3 Å.

[0108] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues set forth in Figure 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.7, 0.5 or 0.3 Å.

[0109] In another embodiment of the invention provides a crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues set forth in Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.45, 0.3 or 0.2 Å.

[0110] In another embodiment of the invention provides a crystalline molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which are identical to JNK3 amino

acid residues set forth in Figure 1, wherein the root mean square deviation between all atoms of said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 1.3, 1.1, 0.9, 0.7 or 0.5 Å.

[0111] In another embodiment of the invention provides a crystalline molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which are identical to JNK3 amino acid residues set forth in Figure 2, wherein the root mean square deviation between all atoms of said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.9, 0.7, 0.5 or 0.3 Å.

[0112] In another embodiment of the invention provides a crystalline molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which are identical to JNK3 amino acid residues set forth in Figure 3, wherein the root mean square deviation between all atoms of said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.8, 0.6, 0.4 or 0.2 Å.

[0113] In yet another embodiment of the invention provides a crystalline molecular complex comprising a protein kinase, wherein the protein kinase comprises a methionine residue that corresponds to Met146 of JNK3, wherein the $\chi 1$ angle is in the range of about -120° to -180° and 45° to 180°. In one embodiment, the protein kinase is a JNK3 protein or a JNK3 homologue. In one embodiment, the $\chi 1$ angle is in the range of -150° to -180°, the $\chi 2$ angle is in the range of -150° to -170°, and the $\chi 3$ angle is in the range of 95° to 135°. In

another embodiment, the $\chi 1$ angle is in the range of 60° to 80°, the $\chi 2$ angle is in the range of 155° to 175°, and the $\chi 3$ angle is in the range of -45° to -65°. In another embodiment, the $\chi 1$ angle is in the range of 135° to 155°, the $\chi 2$ angle is in the range of -115° to -135°, and the $\chi 3$ angle is in the range of -155° to -175°.

Computer Systems

[0114] According to another embodiment, this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the above-mentioned molecules or molecular complexes. In one embodiment, the data defines the above-mentioned binding pockets by comprising the structure coordinates of said amino acid residues according to Figure 1, 2 or 3. To use the structure coordinates generated for JNK3 homologues thereof, or one of its binding pockets, it is at times necessary to convert them into a three-dimensional shape or to generate three-dimensional structural information from them. This is achieved through the use of commercially or publicly available software that is capable of generating a three-dimensional structure of molecules or portions thereof from a set of structure coordinates. In one embodiment, the three-dimensional structure may be displayed as a graphical representation.

[0115] Therefore, according to another embodiment, this invention provides a machine-readable data storage medium comprising a data storage material encoded with machine readable data. In one embodiment, a machine programmed with instructions for using said data, is

capable of generating a three-dimensional structure of any of the molecule or molecular complexes, or binding pockets thereof, that are described herein.

[0116] This invention also provides a computer comprising:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein the data defines any one of the above binding pockets or protein of the molecule or molecular complex;

b) a working memory for storing instructions for processing said machine-readable data;

c) a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for processing said machine readable data as well as an instruction or set of instructions for generating three-dimensional structural information of said binding pocket or protein; and

d) output hardware coupled to the CPU for outputting three-dimensional structural information of the binding pocket or protein, or information produced by using the three-dimensional structural information of said binding pocket or protein. The output hardware may include monitors, touchscreens, printers, facsimile machines, modems, disk drives, CD-ROMs, etc.

[0117] Three-dimensional data generation may be provided by an instruction or set of instructions such as a computer program or commands for generating a three-dimensional structure or graphical representation from structure coordinates, or by subtracting distances between atoms, calculating chemical energies for a JNK3

molecule or molecular complex or homologues thereof, or calculating or minimizing energies for an association of a JNK3 molecule or molecular complex or homologues thereof to a chemical entity. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA [Accelrys ©2001, 2002], O [Jones *et al.*, Acta Crystallogr. A47, pp. 110-119 (1991)] and RIBBONS [Carson, J. Appl. Crystallogr., 24, pp. 9589-961 (1991)], which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described in the Rational Drug Design section.

[0118] Information about said binding pocket or information produced by using said binding pocket can be outputted through display terminals, touchscreens, printers, modems, facsimile machines, CD-ROMs or disk drives. The information can be in graphical or alphanumeric form.

[0119] Figure 9 demonstrates one version of these embodiments. System 10 includes a computer 11 comprising a central processing unit ("CPU") 20, a working memory 22 which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory 24 (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals 26, one or more keyboards 28, one or more input lines 30,

and one or more output lines 40, all of which are interconnected by a conventional bi-directional system bus 50.

[0120] Input hardware 35, coupled to computer 11 by input lines 30, may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems 32 connected by a telephone line or dedicated data line 34. Alternatively or additionally, the input hardware 35 may comprise CD-ROM drives or disk drives 24. In conjunction with display terminal 26, keyboard 28 may also be used as an input device.

[0121] Output hardware 46, coupled to computer 11 by output lines 40, may similarly be implemented by conventional devices. By way of example, output hardware 46 may include CRT display terminal 26 for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA as described herein. Output hardware might also include a printer 42, so that hard copy output may be produced, or a disk drive 24, to store system output for later use. Output hardware may also include a display terminal, a CD or DVD recorder, ZIP™ or JAZ™ drive, or other machine-readable data storage device.

[0122] In operation, CPU 20 coordinates the use of the various input and output devices 35, 46, coordinates data accesses from mass storage 24 and accesses to and from working memory 22, and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to

components of the hardware system 10 are included as appropriate throughout the following description of the data storage medium.

[0123] Figure 10 shows a cross section of a magnetic data storage medium 100 which can be encoded with a machine-readable data that can be carried out by a system such as system 10 of Figure 9. Medium 100 can be a conventional floppy diskette or hard disk, having a suitable substrate 101, which may be conventional, and a suitable coating 102, which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium 100 may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device 24.

[0124] The magnetic domains of coating 102 of medium 100 are polarized or oriented so as to encode in a manner that may be conventional, machine readable data such as that described herein, for execution by a system such as system 10 of Figure 9.

[0125] Figure 11 shows a cross section of an optically-readable data storage medium 110 which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system 10 of Figure 9. Medium 110 can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk that is optically readable and magneto-optically writable. Medium 100 preferably has a suitable substrate 111, which may be conventional, and a suitable coating 112, which may be conventional, usually of one side of substrate 111.

[0126] In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

[0127] In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

[0128] In one embodiment, the structure coordinates of said molecules or molecular complexes are produced by homology modeling of at least a portion of the structure coordinates of Figure 1, 2 or 3. Homology modeling can be used to generate structural models of JNK3 homologues or other homologous proteins based on the known structure of JNK3. This can be achieved by performing one or more of the following steps: performing sequence alignment between the amino acid sequence of an unknown molecule against the amino acid of JNK3; identifying conserved and variable regions by sequence or structure; generating structure co-ordinates for structurally conserved residues of the unknown structure from those of JNK3; generating conformations for the structurally variable residues in the unknown structure; replacing the non-conserved residues of JNK3

with residues in the unknown structure; building side chain conformations; and refining and/or evaluating the unknown structure.

[0129] For example, since the protein sequence of the catalytic domains of JNK3 and JNK1 or JNK2 can be aligned relative to each other, it is possible to construct models of the structures of JNK1 or JNK2, particularly in the regions of the active site, using the JNK3 structure. Software programs that are useful in homology modeling include XALIGN [Wishart, D. S. et al., Comput. Appl. Biosci., 10, pp. 687-88 (1994)] and CLUSTAL W Alignment Tool [Higgins D. G. et al., Methods Enzymol, 266, pp. 383-402 (1996)]. See also, U.S. Patent No. 5,884,230. These references are incorporated herein by reference.

[0130] To perform the sequence alignment, programs such as the "bestfit" program available from the Genetics Computer Group [Waterman in Advances in Applied Mathematics 2, 482 (1981), which is incorporated herein by reference] and CLUSTAL W Alignment Tool [Higgins D. G. et al., Methods Enzymol, 266, pp. 383-402 (1996), which is incorporated by reference] can be used. To model the amino acid side chains of JNK1 or JNK2, the amino acid residues in JNK3 can be replaced, using a computer graphics program such as "O" [Jones et al, (1991) Acta Cryst. Sect. A, 47: 110-119], by those of the homologous protein, where they differ. The same orientation or a different orientation of the amino acid can be used. Insertions and deletions of amino acid residues may be necessary where gaps occur in the sequence alignment. However, certain portions of the active site of JNK3 and its homologues are highly conserved with essentially no insertions and deletions.

[0131] Homology modeling can be performed using, for example, the computer programs SWISS-MODEL available through Glaxo Wellcome Experimental Research in Geneva, Switzerland; WHATIF available on EMBL servers; Schnare et al., J. Mol. Biol, 256: 701-719 (1996); Blundell et al., Nature 326: 347-352 (1987); Fetrow and Bryant, Bio/Technology 11:479-484 (1993); Greer, Methods in Enzymology 202: 239-252 (1991); and Johnson et al, Crit. Rev. Biochem. Mol Biol. 29:1-68 (1994). An example of homology modeling can be found, for example, in Szklarz G.D., Life Sci. 61: 2507-2520 (1997). These references are incorporated herein by reference.

[0132] Thus, in accordance with the present invention, data capable of generating the three dimensional structure of the above molecules or molecular complexes, or binding pockets thereof, can be stored in a machine-readable storage medium, which is capable of displaying three-dimensional structural information or a graphical three-dimensional representation of the structure.

Rational Drug Design

[0133] The JNK3 structure coordinates or the three-dimensional graphical representation generated from these coordinates may be used in conjunction with a computer for a variety of purposes, including drug discovery.

[0134] For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with JNK3 may inhibit or activate JNK3 or its homologues, and are potential drug candidates. Alternatively, the structure encoded by the data may be

displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

[0135] Thus, according to another embodiment, the invention provides a method for designing, selecting and/or optimizing a chemical entity that binds to the molecule or molecular complex comprising the steps of:

(a) providing the structure coordinates of said molecule or molecular complex on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and

(b) designing, selecting and/or optimizing said chemical entity by employing means for performing a fitting operation between said chemical entity and said three-dimensional structural information of said molecule or molecular complex.

[0136] Three-dimensional structural information in step (a) may be generated by instructions such as a computer program or commands that can generate a three-dimensional structure or graphical representation; subtract distances between atoms; calculate chemical energies for a JNK3 molecule, molecular complex or homologues thereof; or calculate or minimize energies of an association of JNK3 molecule, molecular complex or homologues thereof to a chemical entity. These types of computer programs are known in the art. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to

QUANTA [Accelrys ©2001, 2002], O [Jones *et al.*, Acta Crystallogr. A47, pp. 110-119 (1991)] and RIBBONS [Carson, J. Appl. Crystallogr., 24, pp. 9589-961 (1991)], which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described below.

[0137] Another embodiment of the invention provides a method for evaluating the potential of a chemical entity to associate with the molecule or molecular complex as described previously.

[0138] This method comprises the steps of: a) employing computational means to perform a fitting operation between the chemical entity and the molecule or molecular complex described before; b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the molecule or molecular complex; and, optionally, c) outputting said quantified association to a suitable output hardware, such as a CRT display terminal, a CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device, as described previously. The method may further comprise generating a three-dimensional structure, graphical representation thereof, or both, of the molecule or molecular complex prior to step a). In one embodiment, the method is for evaluating the ability of a chemical entity to associate with the binding pocket of a molecule or molecular complex.

[0139] In another embodiment, the method comprises the steps of:

a) constructing a computer model of a binding pocket of the molecule or molecular complex;

b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; de novo ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a JNK3 protein or homologue thereof;

c) employing computational means to perform a fitting program operation between computer models of said chemical entity to be evaluated and said binding pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

d) evaluating the results of said fitting operation to quantify the association between said chemical entity and the binding pocket model, whereby evaluating the ability of said chemical entity to associate with said binding pocket.

[0140] In another embodiment, the invention provides a method of using a computer for evaluating the ability of a chemical entity to associate with the molecule or molecular complex, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and means for generating a three-dimensional graphical representation

of the binding pocket, and wherein said method comprises the steps of:

(a) positioning a first chemical entity within all or part of said binding pocket using a graphical three-dimensional representation of the structure of the chemical entity and the binding pocket;

(b) performing a fitting operation between said chemical entity and said binding pocket by employing computational means;

(c) analyzing the results of said fitting operation to quantitate the association between said chemical entity and all or part of the binding pocket; and

(d) outputting said quantitated association to a suitable output hardware.

[0141] The above method may further comprise the steps of:

(e) repeating steps (a) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that associates with said all or part of said binding pocket based on said quantitated association of said first or second chemical entity.

[0142] Alternatively, the structure coordinates of the JNK3 binding pockets may be utilized in a method for identifying an agonist or antagonist of a molecule comprising a binding pocket of JNK3. This method comprises the steps of:

a) using a three-dimensional structure of the molecule or molecular complex to design, select or optimize a chemical entity;

b) contacting the chemical entity with the molecule or molecular complex;

c) monitoring the catalytic activity of the molecule or molecular complex; and

d) classifying the chemical entity as an agonist or antagonist based on the effect of the chemical entity on the catalytic activity of the molecule or molecular complex.

[0143] In one embodiment, step a) is performed using a graphical representation of the binding pocket or portion thereof of the molecule or molecular complex.

[0144] In another embodiment, the method comprises the steps of:

a) constructing a computer model of a binding pocket of the molecule or molecular complex;

b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; de novo ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a JNK3 protein or homologue thereof;

c) employing computational means to perform a fitting program operation between computer models of said chemical entity to be evaluated and said binding

pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

d) evaluating the results of said fitting operation to quantify the association between said chemical entity and the binding pocket model, whereby evaluating the ability of said chemical entity to associate with said binding pocket;

e) synthesizing said chemical entity; and

f) contacting said chemical entity with said molecule or molecular complex to determine the ability of said compound to activate or inhibit said molecule.

[0145] For the first time, the present invention permits the use of molecular design techniques to identify, select and design chemical entities, including inhibitory compounds, capable of binding to JNK3 or JNK3-like binding pockets, motifs and domains.

[0146] Applicants' elucidation of binding pockets on JNK3 provides the necessary information for designing new chemical entities and compounds that may interact with JNK3 or JNK3-like ATP-binding pockets, in whole or in part. Due to the homology in the kinase core between JNK3, JNK1 and JNK2, compounds that inhibit JNK3 are also expected to inhibit JNK1 and JNK2, especially those compounds that bind the ATP-binding pocket.

[0147] Throughout this section, discussions about the ability of a chemical entity to bind to, associate with or inhibit JNK3 binding pockets refers to features of the entity alone. Assays to determine if a compound

binds to JNK3 are well known in the art and are exemplified below.

[0148] The design of chemical entities that bind to or inhibit JNK3 binding pockets according to this invention generally involves consideration of two factors. First, the entity must be capable of physically and structurally associating with parts or all of the JNK3 binding pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[0149] Second, the entity must be able to assume a conformation that allows it to associate with the JNK3 binding pockets directly. Although certain portions of the entity will not directly participate in these associations, those portions of the entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several chemical entities that directly interact with the JNK3 or JNK3-like binding pockets.

[0150] The potential inhibitory or binding effect of a compound on JNK3 binding pockets may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and the JNK3 binding pockets, testing of the entity is obviated.

However, if computer modeling indicates a strong interaction, the compound may then be synthesized and tested for its ability to bind to a JNK3 binding pocket. This may be achieved by testing the ability of the compound to inhibit JNK3 using the assays described in Example 6. In this manner, synthesis of inoperative compounds may be avoided.

[0151] A potential inhibitor of a JNK3 binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the JNK3 binding pockets.

[0152] One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a JNK3 binding pocket. This process may begin by visual inspection of, for example, a JNK3 binding pocket on the computer screen based on the JNK3 structure coordinates in Figure 1, 2 or 3 or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined *supra*. Docking may be accomplished using software such as QUANTA and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[0153] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID [P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable

Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)]. GRID is available from Oxford University, Oxford, UK.

2. MCSS [A. Miranker *et al.*, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)]. MCSS is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK [D. S. Goodsell *et al.*, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)]. AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK [I. D. Kuntz *et al.*, "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)]. DOCK is available from University of California, San Francisco, CA.

[0154] Once suitable fragments have been selected, they can be assembled into a single compound or complex of compounds. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of JNK3. This would be followed by manual model building using software such as QUANTA or Sybyl [Tripos Associates, St. Louis, MO].

[0155] Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT [P. A. Bartlett *et al.*, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des. , 8, pp. 51-66 (1994)]. CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).

3. HOOK [M. B. Eisen *et al.*, "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19, pp. 199-221 (1994)]. HOOK is available from Molecular Simulations, San Diego, CA.

[0156] Instead of proceeding to build an inhibitor of a JNK3 binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other JNK3 binding compounds may be designed as a whole or "de novo" using either an empty binding pocket or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including:

1. LUDI [H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78

(1992)]. LUDI is available from Molecular Simulations Incorporated, San Diego, CA.

2. LEGEND [Y. Nishibata *et al.*, Tetrahedron, 47, p. 8985 (1991)]. LEGEND is available from Molecular Simulations Incorporated, San Diego, CA.

3. LeapFrog [available from Tripos Associates, St. Louis, MO].

4. SPROUT [V. Gillet *et al.*, "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)]. SPROUT is available from the University of Leeds, UK.

[0157] Other molecular modeling techniques may also be employed in accordance with this invention [see, e.g., N. C. Cohen *et al.*, "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M. Balbes *et al.*, "A Perspective of Modern Methods in Computer-Aided Drug Design", Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology, 4, pp. 777-781 (1994)].

[0158] Once a chemical entity has been designed or selected by the above methods, the efficiency with which that chemical entity may bind to a JNK3 binding pocket may be tested and optimized by computational evaluation. For example, an effective JNK3 binding pocket inhibitor must preferably demonstrate a

relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient JNK3 binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. JNK3 binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

[0159] An entity designed or selected as binding to a JNK3 binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

[0160] Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1995]; AMBER, version 4.1 [P. A. Kollman, University of California at San Francisco, ©1995]; QUANTA/CHARMM [Accelrys, San Diego, CA ©2001, 2002]; Insight II/Discover [Accelrys, San Diego, CA ©2001, 2002]; DelPhi [Accelrys, San Diego, CA ©2001, 2002]; and AMSOL [Quantum Chemistry Program Exchange, Indiana University]. These programs may be implemented, for

instance, using a Silicon Graphics workstation such as an Indigo2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

[0161] Another approach enabled by this invention, is the computational screening of small molecule databases for chemical entities that can bind in whole, or in part, to a JNK3 binding pocket. In this screening, the quality of fit of such entities to the binding pocket may be judged either by shape complementarity or by estimated interaction energy [E. C. Meng *et al.*, J. Comp. Chem., 13, pp. 505-524 (1992)].

[0162] Another particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

[0163] In iterative drug design, crystals of a series of protein or protein complexes are obtained and then the three-dimensional structures of each crystal is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the

protein/compound associations, these associations may be optimized.

[0164] In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. Alternatively, a pre-formed protein crystal is soaked in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

Structure Determination of Other Molecules

[0165] The structure coordinates set forth in Figure 1, 2 or 3 can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

[0166] According to an alternate embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of at least a portion of the structure coordinates set forth in Figure 1, 2 or 3 or homology model thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

[0167] In another embodiment, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray

diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of JNK3 according to Figure 1, 2 or 3 or homology model thereof;

b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex; and

c) instructions for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates.

[0168] For example, the Fourier transform of at least a portion of the structure coordinates set forth in Figure 1, 2 or 3 or homology thereof may be used to determine at least a portion of the structure coordinates of JNK3 homologues or other isoforms of JNK3.

[0169] Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or molecular complex whose structure is unknown comprising the steps of:

a) crystallizing said molecule or molecular complex of unknown structure;

b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

c) applying at least a portion of the structure coordinates set forth in Figure 1, 2 or 3 or homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown; and

d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

[0170] In one embodiment, the method is performed using a computer. In another embodiment, the molecule is selected from the group consisting of JNK3 and JNK3 homologues. In another embodiment, the molecule is a JNK3 molecular complex or homologue thereof.

[0171] By using molecular replacement, all or part of the structure coordinates of the JNK3 as provided by this invention (and set forth in Figure 1, 2 or 3) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*.

[0172] Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the

solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases' for the unknown structure.

[0173] Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the JNK3 according to Figure 1, 2 or 3 or homology model thereof within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

[0174] The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the JNK3 can be resolved by this method.

[0175] In a preferred embodiment, the method of molecular replacement is utilized to obtain structural information about a JNK3 homologue. The structure

coordinates of JNK3 as provided by this invention are particularly useful in solving the structure of JNK3 complexes that are bound by ligands, substrates and inhibitors.

[0176] Furthermore, the structure coordinates of JNK3 as provided by this invention are useful in solving the structure of JNK3 proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "JNK3 mutants", as compared to naturally occurring JNK3). These JNK3 mutants may optionally be crystallized in co-complex with a chemical entity, such an inhibitor or a suicide substrate. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type JNK3. Potential sites for modification within the various binding pockets of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between JNK3 and a chemical entity or compound.

[0177] The structure coordinates are also particularly useful in solving the structure of crystals of JNK3 or JNK3 homologues complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate JNK3 inhibitors. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to those sites can then be

designed and synthesized and tested for their JNK3 inhibition activity.

[0178] All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.2-3.4 Å resolution X-ray data to an R value of about 0.30 or less using computer software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff *et al.*, eds., Academic Press (1985)] or CNS [Brunger et al., Acta Crystallogr. D. Biol. Crystallogr., 54, pp. 905-921, (1998)]. This information may thus be used to optimize known JNK3 inhibitors, and more importantly, to design new JNK3 inhibitors.

[0179] In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

Example 1

Expression and purification of JNK3

[0180] A BLAST search of the EST database using the published JNK3α1 cDNA [S. Gupta et al. (1996)] as a query identified an EST clone (#632588) that contained the entire coding sequence for human JNK3α1. Polymerase chain reactions (PCR) using *pfu* polymerase (Strategene) were used to introduce restriction sites into the cDNA for cloning into the pET-15B expression vector at the NcoI and BamHI sites for expression of the protein in *E. coli*. Due to the poor solubility of

the expressed full length protein (Met 1-Gln 422), an N-terminally truncated protein starting at Ser residue at position 40 (Ser 40), corresponding to Ser 2 of JNK1 and JNK2 proteins [S. Gupta et al. (1996)], preceded by Met (initiation) and Gly residues, were produced. The Gly residue was added in order to introduce an NcoI site for cloning into the expression vector. Further, systematic C-terminal truncations were performed by PCR to identify a construct that gave rise to diffraction-quality crystals. This construct, which was prepared by PCR using deoxyoligonucleotides 5' GCTCTAGAGCTCCATGGGCAGCAAAAGCAAAGTTGACAA 3' (SEQ ID NO: 5)(forward primer with initiation codon underlined) and 5' TAGCGGATCCTCATTCTGAA TTCATTACTTCCTTGTA 3' (SEQ ID NO: 6)(reverse primer with stop codon underlined) as primers and confirmed by DNA sequencing, encodes amino acid residues Ser40-Glu402 of JNK3α1, preceded by Met and Gly residues, was used for structural studies described herein. Control experiments indicated that the truncated JNK3 protein has an equivalent kinase activity towards myelin basic protein when activated with an upstream kinase MKK7 *in vitro*.

[0181] *E.coli* strain BL21 (DE3) (Novagen) transformed with the JNK3 expression construct was grown at 30°C in shaker flasks into log phase (OD600 ~ 0.8) in LB supplemented with 100 μg/ml carbenicillin. IPTG was then added to a final concentration of 0.8 mM and the cells were harvested 2 hours later by centrifugation.

[0182] *E.* coli cell paste containing the truncated JNK3 protein was resuspended in 10 volumes/g lysis buffer [50 mM HEPES, pH 7.2, 10% glycerol (v/v), 100 mM NaCl, 2 mM dithiothreitol (DTT), 0.1mM PMSF, 2 μg/ml

Pepstatin, 1μg/ml each of E-64 and Leupeptin]. Cells were lysed on ice using a microfluidizer and centrifuged at 100,000 x *g* for 30 min at 4°C. The 100,000 x *g* supernatant was diluted 5 fold with Buffer A [20 mM HEPES, pH 7.0, 10% glycerol (v/v), 2 mM DTT) and applied to an SP-Sepharose (Pharmacia) cation-exchange column at 4°C. The column was washed with 5 column volumes of Buffer A, followed by 5 column volumes of Buffer A containing 50 mM NaCl. Bound protein was eluted with a 7.5 column volume linear gradient of 50-300 mM NaCl, and the truncated JNK3 protein was eluted between 150-200 mM NaCl. Eluted JNK3 protein from the SP-Sepharose column was dialyzed at ~ 1 mg/ml against Buffer B [25 mM HEPES, pH 7.0, containing 5% glycerol (v/v), 50 mM NaCl, 10 mM DTT] overnight at 4°C and centrifuged at 3,000 x *g*. The supernatant was concentrated by ultrafiltration (Centriprep-30, Amicon) to 10 mg/ml, centrifuged at 16,000 x *g* and stored at -70°C.

Example 2

Crystallization of JNK3

[0183] Full length human JNK3α1 has a 39-residue extension in the N-terminus when compared to JNK1, JNK2 and other MAP kinases [Fig. 4 and S. Gupta et al. (1996)]. The conserved MAP kinase homologous region of JNK3 without the first 39 residues was used for crystallographic studies. Initial crystallization trials yielded only small crystals that diffracted to 8 Å. Since residues at the C-terminus of Erk2 and p38 are disordered [F. Zhang et al., Nature, 367, pp. 704-11 (1994); K. P. Wilson et al., J. Biol. Chem., 271,

pp. 27696-700 (1996)], it suggests that the C-terminal portions of JNK3 might also be flexible and interfere with the formation of a well-ordered crystal lattice. By combining limited proteolysis and systematic truncation of the protein, an active truncated JNK3 was searched. This screening approach resulted in the growth of larger, well-ordered JNK3 crystals. These crystals were grown from the JNK3 protein lacking the N-terminal 39 and C-terminal 20 residues. The truncated enzyme (residues Ser40-Glu402) displays wild-type kinase activity when activated by MKK7 *in vitro*. All crystallographic studies were carried out using this form of the enzyme.

[0184] Solutions of JNK3-inhibitor complex for crystallization were prepared by incubating the JNK3 protein solution (concentration of 10 mg/ml) with 0.5-1 mM inhibitor for 1 hour at room temperature prior to crystallization. Crystals of JNK3-inhibitor complexes were grown at 20°C by the vapour diffusion hanging-drop method over a reservoir solution containing 18-20% (v/v) polyethylene glycol monomethyl ether (average Mr = 550), 10% (v/v) ethylene glycol, 20 mM β-Mercaptoethanol and 100 mM Hepes (pH 7.0). However, growth of the JNK3-inhibitor crystals required microseeding the freshly made JNK3-inhibitor complex solution with seed stocks prepared from the JNK3-MgAMP-PNP crystals [WO 9957253, incorporated herein by reference]. The seed stock was prepared by crushing JNK3-MgAMP-PNP crystals to obtain a micro-crystal seed stock. The JNK3-inhibitor crystals belong to the orthorhombic space group *P212121* (with one enzyme molecule per asymmetric unit). The solvent content of the crystal is 44%. Before data collection, crystals

were equilibrated in their reservoir solution for 2-5 minutes before flash-frozen in nitrogen gas for X-ray data collection at -170°C.

Example 3

X-Ray data collection and structure determination

[0185] X-ray data were measured on either Raxis IIC or Raxis IV image plate mounted on a Rigaku RU200 rotating-anode generator (Rigaku/MSC). The diffraction images were processed with the program DENZO and data scaled using SCALPACK [Z. Otwinowski, In "Data Collection and Processing", L. Sawyer, N. Isaacs and S.W. Bailey, eds., Warrington, U.K.: Science and Engineering Council/Daresbury Laboratory. pp. 55-62 (1993)]. The data processing statistics are summarized in Table 3.

[0186] The X-ray coordinates of JNK3 from the JNK3-MgAMP-PNP structure [PDB acession number 1JNK] were used as a starting model for refinement of the JNK3-inhibitor complexes. All thermal factors were set to 20.0 $Å^2$. After one round of rigid body and positional refinement, the sigmaA-weighted |Fo|-|Fc| difference electron density maps were calculated using the CNS software package [Brunger et al., Acta Crystallogr. D. Biol. Crystallogr., 54, pp. 905-921, (1998)], and the bound inhibitors were identified. The inhibitor molecules were built and fit to the electron density in the program QUANTA. Then, the JNK3-inhibitor complex models were subjected to torsional dynamics (T=1000 to 4000 °C). Subsequent cycles of model rebuilding, positional refinement, and thermal factor refinement, intercepted with torsional dynamics runs were performed

to obtain the final model. All refinement procedures were carried out using CNS and model building was performed by the program QUANTA. A summary of the diffraction data and refinement statistics is provided in Table 3. The backbone conformation of 85% of the residues is within the most favored regions of the Ramachandran plot, with none in the disallowed region, as defined in the program PROCHECK [R. A. Laskowski et al., J. Appl. Crystallog., 26, pp. 283-91 (1993)].

Table 3

Complex	JNK3-isoxazole1	JNK3-uracil1	JNK3-thiazole1
Data resolution (Å)	2.4	2.2	2.9
Cell parameters	a= 54.75 Å b= 70.48 Å c= 107.66 Å α= 90° β= 90° γ= 90°	a= 51.65 Å b= 71.01 Å c= 106.7 Å α= 90° β= 90° γ= 90°	a= 50.74 Å b= 71.82 Å c= 107.22 Å α= 90° β= 90° γ= 90°
R_{cryst}	23.2	24.1	21.8
R_{free} †	30.5	31.9	29.2

† R_{free} was calculated for a randomly chosen 5% of reflections for JNK3-thiazole1, and a randomly chosen 10% reflections for both JNK3-isoxazole1 and JNK3-uracil1.

[0187] In the final models, disordered residues were not included in the model. Alanine or glycine residues

were used in the model if the side chains of certain residues could not be located in the electron density.

Example 4

Overall Structure

[0188] The crystal structure of JNK3-isoxazole1 includes unphosphorylated JNK3 (residues 44-72, 75-212, 225-372 and 382-400) and isoxazole1. Electron density for residues 40-43, 73-74, 213-224 and 401-402 are missing, and these amino acid residues are presumed disordered. The crystal structure of JNK3-uracil1 includes unphosphorylated JNK3 (residues 45-70, 73-211, 217-373 and 379-400) and uracil1. Electron density for residues 40-44, 71-72, 212-216, 374-378 and 401-402 are missing, and these amino acid residues are presumed disordered. The crystal structure of JNK3-thiazole1 includes unphosphorylated JNK3 (residues 45-72, 77-211, 217-221 and 224-400) and uracil1. Electron density for residues 40-44, 73-76, 212-216, 222-223, and 401-402 are missing, and these amino acid residues are presumed disordered.

[0189] The overall architecture of JNK3 is substantially the same as JNK3 in the JNK3-AMP-PNP complex [WO 9957253] and highly similar to that of Erk2 and p38. However, the conformation in the active site differs. The MAP kinase homologous region of JNK3 (Phe48-Glu397) is 45% identical in amino acid sequence to Erk2 and 51% to p38, whose structures have been reported (F. Zhang et al. (1994); K. P. Wilson et al. (1996); Fig 4). The N-terminal lobe (residues 45-149, and 379-400) of JNK3 contains mostly beta-strands, whereas the C-terminal lobe (residues 150-211, 217-374)

is predominantly alpha-helical. In JNK3, the MAP kinase insertion in the C-terminal domain is 12 residues longer compared to Erk2 and p38, resulting in the N-terminal extension of helix αH and an extra 310 helix, denoted 3/10(2)L14 between αH and α3L14. This 12-residue insertion is referred to as "the JNK insertion" since it is present in all c-Jun N-terminal kinases [S. Gupta et al., (1996)].

Active site

[0190] The active site is situated in a deep cleft between the two domains of JNK3. JNK isoform sequences show that the amino acid residues involved in ATP binding are conserved [Gupta et al., EMBO J. 15, pp. 2760-2770 (1996)]. The catalytic core of protein kinases contains a nucleotide binding sequence Gly-X-Gly-X-X-Gly-X-X that is referred to as "the glycine-rich phosphate anchor loop" due to its structural feature and role in the nucleotide binding [D. R. Knighton et al., Science, 253, pp. 407-13 (1991)]. The conserved Asp189 and Asp207, both are thought to be essential for protein kinase activity [C. S. Gibbs et al., J. Biol. Chem., 267, pp. 4806-10 (1992)].

Inhibitor-binding pocket

[0191] All three compounds bind to the active site of JNK3 (Fig. 8). However, the exact spaces they occupy differ from each other due to the differences in their scaffolds and substituents. The phenyl rings from both uracil1 and isoxazole1 are buried in a hydrophobic pocket formed mainly by Met146 and Lys93, leaving minimal space for additional substituents to the ring. This pocket is normally unavailable when no ligand is

bound in the active site or when the bulky group corresponding to the phenyl ring in uracil1 and isoxazole1 is not present in the bound ligand, such as with ATP, AMP-PNP or thiazole1.

[0192] As illustrated in Figure 6, the binding of uracil1 induces a flip in the orientation of Met146. In order to avoid the clash with the phenyl group of uracil1, the Met146 takes a different conformation to accommodate the inhibitor. Compared to the Met146 in the JNK3-AMP-PNP structure, when viewed along the Cα-Cβ bond, the Cγ of Met146 in JNK3-uracil1 and JNK3-isoxazole1 swing about 110° clockwise, and about 125° counter clockwise, respectively. This conformational change results in the movement of Ile124 and Ser125 in the inhibitor binding-pocket, which further affects the conformation of other surrounding residues Asn101 to Cys117. Helix C (Figure 6) undergoes a pivoting movement around its N-terminus, and the C-terminal portion of Helix C swings out about 3 Å as a result of the movement in Ile124. The movement of helix C results in the disruption of the salt bridge between Glu111 of Helix C and Lys93 of the active site. This salt bridge is required for ATP hydrolysis.

[0193] In the JNK3-isoxazole1 and JNK3-uracil1 complexes, the backbone atoms of Lys93, Ile124, Leu126, Leu144 and Met146 are altered compared to those in the JNK3-AMP-PNP crystal structure. Table 4 shows a comparison of the dihedral angles for those residues. As will be understood by those skilled in the art, the ϕ_n angle refers to the rotation around the bond between the alpha carbon and the nitrogen, and the Ψ_n angle refers to the rotation around the bond between the carbonyl carbon and the alpha carbon. The subscript

"n" identifies the amino acid whose conformation is being described [for a general reference, see Blundell and Johnson, Protein Crystallography, Academic Press, London, 1976].

Table 4

Protein/(ϕ, Ψ)°	Lys93	Ile124	Leu126	Leu144	Met146
JNK3-AMP-PNP	-109, 129	-43, 134	-95, 130	-99, 127	-134, 171
JNK3-isoxazole1	-135, 130	-62, 129	-72, 120	-122, 127	-157, 174
JNK3-uracil1	-114, 129	-58, 137	-95, 136	-110, 143	-143, 162
P38α-apo	-106, 125	-59, 141	-90, 120	-122, 139	-137, 174
P38α-compound	-106, 130	-64, 138	-99, 122	-119, 137	-143, 169

The ϕ, Ψ angles of Met146 for the JNK3-thiazole1 complex are -124° and -171°, respectively.

[0194] In addition, the number of hydrogen bonds and contacts that these compounds make with JNK3 are also different from each other (Fig. 8). In the case of AMP-PNP, the adenine base of the nucleotide is bound in the back of the domain interface, forming two hydrogen bonds to the protein backbone atoms in the hinge region. The amino group (N6) forms a hydrogen bond to the backbone carbonyl of Glu147 ("H-bond I"), and N1 accepts a proton from the backbone amide of Met149 ("H-bond II"). As shown in Fig. 8, H-bond II is present in

all three JNK3-inhibitor complexes, with the one in JNK3 uracil1 complex mediated by a water molecule. H-bond I is only present in the JNK3-isoxazole1 complex, where the aromatic carbon from the pyrimidine ring donates a proton to the backbone carbonyl of Glu147. Additionally, both isoxazole1 and uracil1 form hydrogen bonds with the backbone carbonyl of Met149.

Example 5

The Use of JNK3-inhibitor Coordinates for Inhibitor Design

[0195] The coordinates of Figure 1, 2 and 3 were used to design compounds, including inhibitory compounds, that associate with JNK3 or homologues of JNK3. This process was aided by using a computer comprising a machine-readable data storage medium encoded with a set of machine-executable instructions, wherein the recorded instructions are capable of displaying a three-dimensional representation of the JNK3-inhibitor complex or a portion thereof.

[0196] Results from enzyme assays have shown that among the three compounds, thiazole1 is the poorest inhibitor of JNK3 (Ki=13 μM), while uracil1 and isoxazole1 are quite comparable to each other (~0.8 μM). Our structural studies showed that the main difference between thiazole1 and the other compounds is its lack of a bulky substituent accessing the hydrophobic pocket, indicating the importance of retaining such bulky substituents for achieving high potency. Furthermore, isoxazole1 is the smallest molecule among the three compounds. While isoxazole1

occupies the least space in the active site, it sits closest to the protein and thereby makes the greatest number of direct hydrogen bonds. Therefore, it may be most advantageous to select isoxazole1 as the lead molecule for optimization.

[0197] Structural comparison revealed that several subsites occupied by thiazole1 and uracil1 are not accessed by isoxazole1. Although thiazole1 and uracil1 make fewer direct contacts with the JNK3 protein (Fig. 8), the additional subsites they occupy may contribute to their binding affinities. This suggests that modifications of isoxazole1 to access these subsites might help to further improve its potency. The subsite identified in the JNK3-thiazole1 structure consists of residues Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155. These residues were in direct contact with thiazole-2-yl-pyridine of thiazole1 and phenyl of uracil1 (Fig. 7B). This subsite is at the entrance of the active site and is partially exposed to the solvent, indicating that it might be possible to improve the potency as well as the solubility of isoxazole1 by accessing this structurally important subsite. When the acetaldehyde of isoxazole1 was replaced by a bulky group such as a phenyl group or a cyclohexyl group, the potency improved significantly. The subsite identified in the JNK3-uracil1 structure consists of residues Ser72, Ser193 and Asn152. These residues surround the pyrimidine-2,4-dione group of uracil1 and the ribose group of AMP-PNP (Fig. 7C), suggesting that additional substitutions at O1 of isoxazole1 and/or modification of the 5-methyl may be helpful for further improving the properties of isoxazole1-derived ligands.

[0198] The above example illustrates how structural information from different JNK3-inhibitor complexes can be used to design a better class of compounds.

Example 6

JNK3 Activity Inhibition Assay

A. JNK3 activation

[0199] Five mg of JNK3 was diluted to 0.5 mg/ml in 50 mM HEPES buffer, pH 7.5, containing 100 mM NaCl, 5 mM DTT, 20 mM $MgCl_2$, 1 mM ATP. GST-MKK7(DD) kinase (the upstream mutant form of one of the activating kinases of JNK3) was added at a molar ratio of 1 GST-MKK7:2.5 JNK3. After 30 min at 25°C the reaction mixture was concentrated 5-fold by ultrafiltration in a Centriprep-30 (Amicon, Beverly, MA), then diluted back up to 10 ml and an additional 1 mM ATP added. This procedure was repeated three times to remove ADP and replenish ATP. The final (third) addition of ATP was 5 mM and the mixture incubated overnight at 4°C.

[0200] The activated JNK3/GST-MKK7(DD) reaction mixture was exchanged into 50 mM HEPES buffer, pH 7.5, containing 5 mM DTT and 5% glycerol (w/v) by dialysis or ultrafiltration. The reaction mixture was adjusted to 1.1 M potassium phosphate, pH 7.5, and purified by hydrophobic interactions chromatography (at 25°C) using a Rainin Hydropore column. GST-MKK7 and unactivated JNK3 do not bind under these conditions and when a 1.1 to 0.05 M potassium phosphate gradient is developed over 60 min at a flow rate of 1 ml/min, doubly phosphorylated JNK3 is separated from singly phosphorylated JNK3.

[0201] Activated JNK3 (i.e. doubly phosphorylated) was stored at -70°C at 0.25-1 mg/ml.

B. JNK3 Inhibition Assay

[0202] To determine the IC_{50} of the compound binding to JNK3, the kinase activity of JNK3 was monitored by a coupled enzyme assay. In this assay, for every molecule of ADP generated by the JNK3 kinase activity one molecule of NADH is converted to NAD which can be conveniently monitored as an absorbance decrease at 340 nm. The following are the final concentrations of various reagents used in the assay: 100 mM HEPES buffer, pH 7.6, 10 mM $MgCl_2$, 25 mM β-glycerophosphate, 30 μM ATP, 2 mM phosphoenolpyruvate, 2 μM pyruvate kinase, 2 μM lactate dehydrogenase, 200 μM NADH, 200 μM EGF receptor peptide KRELVEPLTPSGEAPNQALLR (SEQ ID NO: 7), and 10 nM activated JNK3. First, all of the above reagents with the exception of ATP were mixed and 175 μl aliquots were placed per well in a 96-well plate. A 5 μl DMSO solution of the compound was added to each well, mixed, and allowed to stand at 30°C for 10 minutes. Typically about 10 different concentrations of the compound were tested. The reactions were initiated with the addition of 20 μl of ATP solution. Absorbance change at 340 nm were monitored as a function of time. IC_{50} was obtained by fitting the rates vs. compound concentration data to a simple competitive inhibition model.

[0203] While we have described a number of embodiments of this invention, it is apparent that our basic constructions may be altered to provide other embodiments that utilize the products, processes and methods of this invention. Therefore, it will be

appreciated that the scope of this invention is to be defined by the appended claims, rather than by the specific embodiments that have been presented by way of example.

We claim:

1. A crystal comprising:

a) a JNK3 protein or homologue thereof; and

b) an inhibitor that is capable of inducing the Met146 in JNK3 or corresponding methionine in the JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180° upon binding.

2. A crystal comprising:

a) a JNK3 protein or homologue thereof; and

b) an inhibitor selected from the group consisting of N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide, 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid phenylamide, 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide, 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol and 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide.

3. The crystal of claim 1 or 2 which is capable of diffracting X-rays to at least 3.0 Å.

4. The crystal according to claim 1 or 2, wherein the JNK3 protein or homologue thereof is phosphorylated or unphosphorylated.

5. The crystal according to claim 1 or 2, wherein the JNK3 protein is JNK3$\alpha 1$.

6. The crystal according to claim 1 or 2, wherein the JNK3 protein or JNK3 homologue contains a C-terminal deletion of about 20 amino acid residues.

7. The crystal according to claim 1 or 2, wherein the JNK3 protein has an N-terminal deletion of about 40 amino acid residues.

8. A method of producing a JNK3-inhibitor complex crystal or JNK3 homologue-inhibitor complex crystal, comprising the steps of:

a) producing a composition comprising a crystallization solution and a JNK3 protein or homologue thereof complexed with an inhibitor, wherein the inhibitor is capable of inducing the Met146 in the JNK3 protein or corresponding methionine in the JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180°; and

b) subjecting said composition to devices or conditions which promote crystallization.

9. The method of claim 8, wherein the composition is treated with micro-crystals of JNK3 protein, JNK3 protein complexes or homologues thereof after step a) but prior to step b).

10. A crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Lys93, Ile124, Leu126, Leu144, Met146 according to Figure 1 or 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues

of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.3 Å.

11. A crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155 according to Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 1.0 Å.

12. A crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues set forth in Figure 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.9 Å.

13. A crystalline molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which are identical to JNK3 amino acid residues set forth in Figure 1, wherein the root mean square deviation between all atoms of said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 1.3 Å.

14. A crystalline molecular complex comprising a protein kinase, wherein the protein kinase comprises a methionine residue that corresponds to

Met146 of JNK3, wherein the residue has a $\chi 1$ angle in the range of about -120° to -180° and 45° to 180°.

15. The crystalline molecular complex of claim 14, wherein the $\chi 1$ angle is in the range of -150° to -180°, the $\chi 2$ angle is in the range of -150° to -170°, and the $\chi 3$ angle is in the range of 95° to 135°.

16. The crystalline molecular complex of claim 14, wherein the $\chi 1$ angle is in the range of 60° to 80°, the $\chi 2$ angle is in the range of 155° to 175°, and the $\chi 3$ angle is in the range of -45° to -65°.

17. The crystalline molecular complex of claim 14, wherein the $\chi 1$ angle is in the range of 135° to 155°, the $\chi 2$ angle is in the range of -115° to -135°, and the $\chi 3$ angle is in the range of -155° to -175°.

18. The crystalline molecule or molecular complex according to any one of claims 10-17, wherein the molecule or molecular complex is a JNK3 protein or JNK3 protein complex, or homologues thereof.

19. A computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the binding pocket according to any one of claims 10-11 or the protein according to any one of claims 12-17;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-

readable data and means for generating three-dimensional structural information of said binding pocket or protein; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or protein, or information produced using said three-dimensional structural information of said binding pocket or protein.

20. The computer according to claim 19, wherein said data is produced by homology modeling of at least a portion of the structure coordinates of Figure 1, 2 or 3.

21. The computer according to claim 19, wherein said means for generating three-dimensional structural information is provided by means for generating a three-dimensional graphical representation of said binding pocket or protein.

22. The computer according to claim 19, wherein said output hardware is a display terminal, a printer, CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device.

23. A method for designing, selecting and/or optimizing a chemical entity that binds to the molecule or molecular complex according to any one of the claims 10-17 comprising the steps of:

(a) providing the structure coordinates of said molecule or molecular complex on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and

(b) designing, selecting and/or optimizing said chemical entity by performing a fitting operation between said chemical entity and said three-dimensional structural information of said molecule or molecular complex.

24. A method for evaluating the ability of a chemical entity to associate with the molecule or molecular complex according to any one of claims 10-17 comprising the steps of:

(a) employing computational means to perform a fitting operation between the chemical entity and the molecule or molecular complex; and

(b) analyzing the results of said fitting operation to quantitate the association between the chemical entity and the molecule or molecular complex.

25. The method according to claim 24, further comprising generating a three-dimensional graphical representation of the molecule or molecular complex prior to step (a).

26. The method of claim 24, wherein the method is for evaluating the ability of a chemical entity to associate with the binding pocket of the molecule or molecular complex.

27. A method of using a computer for evaluating the ability of a chemical entity to associate with the molecule or molecular complex according to any one of claims 10-17, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket

or protein and means for generating a three-dimensional graphical representation of the binding pocket or protein, and wherein said method comprises the steps of:

(a) positioning a first chemical entity within all or part of said binding pocket or protein using a graphical three-dimensional representation of the structure of the chemical entity and the binding pocket or protein;

(b) performing a fitting operation between said chemical entity and said binding pocket or protein by employing computational means;

(c) analyzing the results of said fitting operation to quantitate the association between said chemical entity and all or part of the binding pocket or protein; and

(d) outputting said quantitated association to suitable output hardware.

28. The method according to claim 27, further comprising the steps of:

(e) repeating steps (a) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that associates with said all or part of said binding pocket or protein based on said quantitated association of said first or second chemical entity.

29. A method for identifying an agonist or antagonist of a molecule or molecular complex according to any one of claims 10-17 comprising the steps of:

(a) using a three-dimensional structure of the molecule or molecular complex to design or select a chemical entity;

(b) contacting the chemical entity with the molecule or the molecular complex;

(c) monitoring the catalytic activity of the molecule or molecular complex; and

(d) classifying the chemical entity as an agonist or antagonist based on the effect of the chemical entity on the catalytic activity of the molecule or molecular complex.

30. A method of utilizing molecular replacement to obtain a structural model of a molecule or a molecular complex of unknown structure, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex;

(c) applying at least a portion of the structure coordinates set forth in Figure 1, 2 or 3 or in a homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

31. The method according to claim 30, wherein the molecule is a JNK3 protein or homologue thereof.

32. The method according to claim 30, wherein the molecular complex is selected from the group consisting of a JNK3 protein complex and a JNK3 homologue complex.

ABSTRACT

[0204] The invention relates to crystalline molecules or molecular complexes that comprise binding pockets of c-Jun N-terminal kinase 3 (JNK3) or its homologues. The invention also relates to crystals comprising JNK3 and an inhibitor. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of JNK3 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the molecule or molecular complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compounds, including agonists and antagonists, which bind to JNK3 or homologues thereof.

FIG. 1A

	Atom	Type	Resid	#	X	Y	Z	Occ	B
ATOM	1	CB	VAL	44	-1.554	11.775	58.841	1.00	44.68
ATOM	2	CG1	VAL	44	-0.373	12.518	59.504	1.00	41.59
ATOM	3	CG2	VAL	44	-2.770	12.693	58.662	1.00	38.80
ATOM	4	C	VAL	44	-0.036	11.928	56.766	1.00	45.09
ATOM	5	O	VAL	44	0.936	11.355	56.264	1.00	41.95
ATOM	6	N	VAL	44	-0.692	9.711	57.661	1.00	46.59
ATOM	7	CA	VAL	44	-1.140	11.123	57.467	1.00	45.20
ATOM	8	N	ASP	45	-0.196	13.252	56.744	1.00	45.56
ATOM	9	CA	ASP	45	0.749	14.177	56.127	1.00	46.19
ATOM	10	CB	ASP	45	0.318	15.615	56.445	1.00	50.81
ATOM	11	CG	ASP	45	0.477	16.559	55.257	1.00	54.31
ATOM	12	OD1	ASP	45	1.579	16.604	54.657	1.00	54.34
ATOM	13	OD2	ASP	45	-0.504	17.269	54.936	1.00	53.14
ATOM	14	C	ASP	45	2.222	13.969	56.530	1.00	45.23
ATOM	15	O	ASP	45	3.125	14.433	55.832	1.00	41.27
ATOM	16	N	ASN	46	2.459	13.286	57.654	1.00	44.70
ATOM	17	CA	ASN	46	3.816	13.018	58.127	1.00	40.32
ATOM	18	CB	ASN	46	3.821	12.654	59.616	1.00	44.41
ATOM	19	CG	ASN	46	2.903	11.483	59.953	1.00	48.13
ATOM	20	OD1	ASN	46	2.249	10.903	59.080	1.00	51.07
ATOM	21	ND2	ASN	46	2.836	11.147	61.233	1.00	47.12
ATOM	22	C	ASN	46	4.511	11.933	57.311	1.00	37.04
ATOM	23	O	ASN	46	5.742	11.873	57.257	1.00	33.54
ATOM	24	N	GLN	47	3.715	11.069	56.690	1.00	31.75
ATOM	25	CA	GLN	47	4.253	10.008	55.855	1.00	32.28
ATOM	26	CB	GLN	47	3.180	8.964	55.586	1.00	32.94
ATOM	27	CG	GLN	47	2.635	8.292	56.827	1.00	35.16
ATOM	28	CD	GLN	47	1.600	7.245	56.492	1.00	37.29
ATOM	29	OE1	GLN	47	0.412	7.411	56.777	1.00	39.51
ATOM	30	NE2	GLN	47	2.042	6.161	55.861	1.00	38.10
ATOM	31	C	GLN	47	4.720	10.608	54.527	1.00	32.61
ATOM	32	O	GLN	47	5.560	10.031	53.823	1.00	34.45
ATOM	33	N	PHE	48	4.156	11.770	54.202	1.00	30.02
ATOM	34	CA	PHE	48	4.458	12.503	52.977	1.00	24.00
ATOM	35	CB	PHE	48	3.173	13.045	52.364	1.00	19.63
ATOM	36	CG	PHE	48	2.188	11.982	51.986	1.00	23.41
ATOM	37	CD1	PHE	48	1.336	11.442	52.942	1.00	18.66
ATOM	38	CD2	PHE	48	2.089	11.541	50.664	1.00	23.94
ATOM	39	CE1	PHE	48	0.391	10.471	52.596	1.00	20.60
ATOM	40	CE2	PHE	48	1.149	10.569	50.294	1.00	18.66
ATOM	41	CZ	PHE	48	0.292	10.032	51.266	1.00	23.76
ATOM	42	C	PHE	48	5.387	13.682	53.235	1.00	22.48
ATOM	43	O	PHE	48	5.876	13.876	54.346	1.00	27.78
ATOM	44	N	TYR	49	5.659	14.434	52.173	1.00	19.53
ATOM	45	CA	TYR	49	6.493	15.620	52.225	1.00	15.88
ATOM	46	CB	TYR	49	7.939	15.255	52.551	1.00	11.81
ATOM	47	CG	TYR	49	8.848	14.994	51.384	1.00	16.74
ATOM	48	CD1	TYR	49	9.885	15.869	51.093	1.00	21.41
ATOM	49	CE1	TYR	49	10.800	15.595	50.073	1.00	22.47
ATOM	50	CD2	TYR	49	8.735	13.837	50.622	1.00	20.14
ATOM	51	CE2	TYR	49	9.653	13.555	49.594	1.00	20.86
ATOM	52	CZ	TYR	49	10.681	14.436	49.332	1.00	22.92
ATOM	53	OH	TYR	49	11.617	14.156	48.361	1.00	25.56
ATOM	54	C	TYR	49	6.376	16.346	50.892	1.00	20.03
ATOM	55	O	TYR	49	6.214	15.715	49.847	1.00	21.71
ATOM	56	N	SER	50	6.441	17.673	50.934	1.00	18.79
ATOM	57	CA	SER	50	6.301	18.486	49.733	1.00	14.86

FIG. 1B

ATOM	58	CB	SER	50	5.456	19.723	50.017	1.00	15.67
ATOM	59	OG	SER	50	4.087	19.385	50.146	1.00	17.38
ATOM	60	C	SER	50	7.577	18.909	49.048	1.00	18.39
ATOM	61	O	SER	50	8.606	19.149	49.685	1.00	18.03
ATOM	62	N	VAL	51	7.494	18.983	47.723	1.00	23.30
ATOM	63	CA	VAL	51	8.614	19.396	46.894	1.00	27.03
ATOM	64	CB	VAL	51	9.213	18.217	46.082	1.00	27.90
ATOM	65	CG1	VAL	51	10.674	18.504	45.755	1.00	30.77
ATOM	66	CG2	VAL	51	9.088	16.907	46.852	1.00	31.13
ATOM	67	C	VAL	51	8.104	20.459	45.931	1.00	27.87
ATOM	68	O	VAL	51	6.958	20.400	45.476	1.00	29.93
ATOM	69	N	GLU	52	8.930	21.468	45.672	1.00	29.63
ATOM	70	CA	GLU	52	8.543	22.538	44.757	1.00	27.26
ATOM	71	CB	GLU	52	9.072	23.897	45.221	1.00	29.95
ATOM	72	CG	GLU	52	8.638	25.037	44.300	1.00	36.89
ATOM	73	CD	GLU	52	9.302	26.360	44.619	1.00	39.00
ATOM	74	OE1	GLU	52	8.691	27.156	45.363	1.00	41.58
ATOM	75	OE2	GLU	52	10.421	26.602	44.112	1.00	35.61
ATOM	76	C	GLU	52	9.072	22.253	43.367	1.00	22.35
ATOM	77	O	GLU	52	10.276	22.284	43.135	1.00	25.69
ATOM	78	N	VAL	53	8.167	21.946	42.450	1.00	20.71
ATOM	79	CA	VAL	53	8.533	21.672	41.070	1.00	22.02
ATOM	80	CB	VAL	53	8.191	20.215	40.679	1.00	21.57
ATOM	81	CG1	VAL	53	8.531	19.970	39.223	1.00	24.78
ATOM	82	CG2	VAL	53	8.968	19.238	41.558	1.00	24.81
ATOM	83	C	VAL	53	7.819	22.668	40.148	1.00	23.76
ATOM	84	O	VAL	53	6.686	22.434	39.700	1.00	24.98
ATOM	85	N	GLY	54	8.471	23.803	39.909	1.00	15.00
ATOM	86	CA	GLY	54	7.892	24.820	39.057	1.00	12.96
ATOM	87	C	GLY	54	6.635	25.424	39.651	1.00	12.55
ATOM	88	O	GLY	54	6.643	25.866	40.789	1.00	16.27
ATOM	89	N	ASP	55	5.557	25.462	38.870	1.00	18.77
ATOM	90	CA	ASP	55	4.285	26.024	39.335	1.00	19.62
ATOM	91	CB	ASP	55	3.300	26.271	38.176	1.00	23.42
ATOM	92	CG	ASP	55	3.773	27.322	37.175	1.00	28.63
ATOM	93	OD1	ASP	55	4.643	28.158	37.505	1.00	29.48
ATOM	94	OD2	ASP	55	3.232	27.317	36.045	1.00	24.85
ATOM	95	C	ASP	55	3.607	25.044	40.261	1.00	17.02
ATOM	96	O	ASP	55	2.596	25.368	40.876	1.00	18.70
ATOM	97	N	SER	56	4.128	23.823	40.288	1.00	19.63
ATOM	98	CA	SER	56	3.560	22.747	41.086	1.00	20.49
ATOM	99	CB	SER	56	3.424	21.502	40.197	1.00	19.15
ATOM	100	OG	SER	56	2.680	21.805	39.034	1.00	21.54
ATOM	101	C	SER	56	4.283	22.372	42.380	1.00	14.16
ATOM	102	O	SER	56	5.471	22.639	42.565	1.00	10.18
ATOM	103	N	THR	57	3.533	21.754	43.281	1.00	11.32
ATOM	104	CA	THR	57	4.083	21.282	44.539	1.00	15.55
ATOM	105	CB	THR	57	3.360	21.910	45.778	1.00	15.32
ATOM	106	OG1	THR	57	3.485	23.339	45.751	1.00	17.52
ATOM	107	CG2	THR	57	3.965	21.395	47.065	1.00	8.74
ATOM	108	C	THR	57	3.860	19.770	44.550	1.00	11.87
ATOM	109	O	THR	57	2.720	19.307	44.476	1.00	8.37
ATOM	110	N	PHE	58	4.945	19.006	44.542	1.00	9.07
ATOM	111	CA	PHE	58	4.836	17.553	44.592	1.00	15.67
ATOM	112	CB	PHE	58	5.958	16.891	43.795	1.00	20.52
ATOM	113	CG	PHE	58	5.601	16.620	42.357	1.00	25.17
ATOM	114	CD1	PHE	58	5.240	17.660	41.506	1.00	29.63
ATOM	115	CD2	PHE	58	5.631	15.324	41.852	1.00	29.62
ATOM	116	CE1	PHE	58	4.914	17.411	40.160	1.00	31.71

FIG. 1C

ATOM	117	CE2	PHE	58	5.309	15.058	40.510	1.00	24.12
ATOM	118	CZ	PHE	58	4.949	16.104	39.663	1.00	25.51
ATOM	119	C	PHE	58	4.851	17.031	46.029	1.00	15.98
ATOM	120	O	PHE	58	5.895	17.015	46.684	1.00	13.06
ATOM	121	N	THR	59	3.676	16.667	46.531	1.00	18.04
ATOM	122	CA	THR	59	3.524	16.115	47.878	1.00	16.76
ATOM	123	CB	THR	59	2.194	16.572	48.489	1.00	22.41
ATOM	124	OG1	THR	59	2.113	18.003	48.419	1.00	26.00
ATOM	125	CG2	THR	59	2.080	16.134	49.939	1.00	24.02
ATOM	126	C	THR	59	3.584	14.575	47.792	1.00	12.75
ATOM	127	O	THR	59	2.572	13.904	47.586	1.00	6.67
ATOM	128	N	VAL	60	4.783	14.020	47.938	1.00	12.07
ATOM	129	CA	VAL	60	4.975	12.572	47.821	1.00	16.39
ATOM	130	CB	VAL	60	5.977	12.234	46.675	1.00	9.02
ATOM	131	CG1	VAL	60	5.416	12.643	45.336	1.00	11.33
ATOM	132	CG2	VAL	60	7.307	12.913	46.914	1.00	2.00
ATOM	133	C	VAL	60	5.435	11.813	49.076	1.00	20.62
ATOM	134	O	VAL	60	5.896	12.397	50.057	1.00	24.40
ATOM	135	N	LEU	61	5.317	10.491	49.015	1.00	18.08
ATOM	136	CA	LEU	61	5.736	9.632	50.111	1.00	14.84
ATOM	137	CB	LEU	61	5.429	8.166	49.790	1.00	12.15
ATOM	138	CG	LEU	61	3.962	7.752	49.646	1.00	10.77
ATOM	139	CD1	LEU	61	3.888	6.332	49.096	1.00	8.34
ATOM	140	CD2	LEU	61	3.265	7.851	50.981	1.00	5.08
ATOM	141	C	LEU	61	7.235	9.799	50.292	1.00	13.78
ATOM	142	O	LEU	61	7.968	9.936	49.318	1.00	15.00
ATOM	143	N	LYS	62	7.683	9.750	51.541	1.00	13.56
ATOM	144	CA	LYS	62	9.088	9.903	51.888	1.00	11.45
ATOM	145	CB	LYS	62	9.232	9.898	53.408	1.00	18.13
ATOM	146	CG	LYS	62	8.642	11.124	54.072	1.00	25.67
ATOM	147	CD	LYS	62	8.801	11.061	55.587	1.00	33.51
ATOM	148	CE	LYS	62	8.556	12.419	56.243	1.00	35.54
ATOM	149	NZ	LYS	62	8.729	12.377	57.734	1.00	42.33
ATOM	150	C	LYS	62	10.068	8.918	51.253	1.00	7.12
ATOM	151	O	LYS	62	11.291	9.085	51.362	1.00	4.58
ATOM	152	N	ARG	63	9.540	7.882	50.610	1.00	11.02
ATOM	153	CA	ARG	63	10.382	6.884	49.942	1.00	10.76
ATOM	154	CB	ARG	63	9.583	5.598	49.667	1.00	9.20
ATOM	155	CG	ARG	63	8.343	5.763	48.797	1.00	10.52
ATOM	156	CD	ARG	63	7.573	4.449	48.599	1.00	13.21
ATOM	157	NE	ARG	63	8.381	3.390	47.986	1.00	9.08
ATOM	158	CZ	ARG	63	7.891	2.244	47.514	1.00	8.35
ATOM	159	NH1	ARG	63	6.594	1.982	47.569	1.00	4.31
ATOM	160	NH2	ARG	63	8.710	1.344	46.992	1.00	6.68
ATOM	161	C	ARG	63	10.943	7.453	48.637	1.00	8.74
ATOM	162	O	ARG	63	12.047	7.115	48.229	1.00	7.79
ATOM	163	N	TYR	64	10.193	8.367	48.034	1.00	9.03
ATOM	164	CA	TYR	64	10.570	9.010	46.786	1.00	11.96
ATOM	165	CB	TYR	64	9.301	9.451	46.068	1.00	7.77
ATOM	166	CG	TYR	64	8.389	8.297	45.771	1.00	2.00
ATOM	167	CD1	TYR	64	8.878	7.155	45.151	1.00	2.00
ATOM	168	CE1	TYR	64	8.058	6.074	44.883	1.00	2.11
ATOM	169	CD2	TYR	64	7.042	8.328	46.120	1.00	2.00
ATOM	170	CE2	TYR	64	6.212	7.246	45.852	1.00	2.00
ATOM	171	CZ	TYR	64	6.731	6.119	45.234	1.00	6.29
ATOM	172	OH	TYR	64	5.931	5.032	44.955	1.00	11.87
ATOM	173	C	TYR	64	11.455	10.202	47.081	1.00	15.27
ATOM	174	O	TYR	64	10.971	11.288	47.394	1.00	19.73
ATOM	175	N	GLN	65	12.759	10.004	46.980	1.00	17.91

FIG. 1D

ATOM	176	CA	GLN	65	13.704	11.070	47.285	1.00	19.85
ATOM	177	CB	GLN	65	14.856	10.480	48.109	1.00	16.92
ATOM	178	CG	GLN	65	14.366	9.720	49.332	1.00	21.05
ATOM	179	CD	GLN	65	15.462	8.956	50.046	1.00	29.96
ATOM	180	OE1	GLN	65	16.641	9.021	49.674	1.00	32.66
ATOM	181	NE2	GLN	65	15.081	8.231	51.091	1.00	32.03
ATOM	182	C	GLN	65	14.251	11.886	46.104	1.00	21.54
ATOM	183	O	GLN	65	14.269	11.430	44.966	1.00	26.33
ATOM	184	N	ALA	66	14.658	13.119	46.402	1.00	23.53
ATOM	185	CA	ALA	66	15.252	14.051	45.435	1.00	21.77
ATOM	186	CB	ALA	66	16.727	13.720	45.233	1.00	19.86
ATOM	187	C	ALA	66	14.573	14.204	44.078	1.00	17.68
ATOM	188	O	ALA	66	15.211	13.988	43.057	1.00	16.11
ATOM	189	N	LEU	67	13.322	14.656	44.061	1.00	15.00
ATOM	190	CA	LEU	67	12.600	14.829	42.805	1.00	14.02
ATOM	191	CB	LEU	67	11.111	15.059	43.056	1.00	4.58
ATOM	192	CG	LEU	67	10.370	14.361	44.185	1.00	2.00
ATOM	193	CD1	LEU	67	8.880	14.471	43.920	1.00	2.00
ATOM	194	CD2	LEU	67	10.789	12.921	44.291	1.00	4.73
ATOM	195	C	LEU	67	13.105	15.981	41.917	1.00	21.98
ATOM	196	O	LEU	67	13.107	17.146	42.330	1.00	26.10
ATOM	197	N	ALA	68	13.520	15.652	40.697	1.00	23.28
ATOM	198	CA	ALA	68	13.972	16.653	39.736	1.00	20.49
ATOM	199	CB	ALA	68	15.337	16.268	39.178	1.00	14.57
ATOM	200	C	ALA	68	12.906	16.677	38.631	1.00	23.80
ATOM	201	O	ALA	68	12.214	15.689	38.416	1.00	21.05
ATOM	202	N	PRO	69	12.707	17.826	37.966	1.00	28.37
ATOM	203	CD	PRO	69	13.222	19.182	38.224	1.00	31.49
ATOM	204	CA	PRO	69	11.687	17.858	36.914	1.00	27.06
ATOM	205	CB	PRO	69	11.486	19.359	36.669	1.00	28.04
ATOM	206	CG	PRO	69	12.005	20.022	37.932	1.00	28.91
ATOM	207	C	PRO	69	12.140	17.175	35.633	1.00	28.24
ATOM	208	O	PRO	69	13.341	17.043	35.364	1.00	23.40
ATOM	209	N	ILE	70	11.153	16.705	34.874	1.00	31.91
ATOM	210	CA	ILE	70	11.355	16.052	33.580	1.00	38.18
ATOM	211	CB	ILE	70	10.869	14.587	33.607	1.00	34.66
ATOM	212	CG2	ILE	70	10.114	14.234	32.338	1.00	36.72
ATOM	213	CG1	ILE	70	12.073	13.670	33.822	1.00	31.51
ATOM	214	CD1	ILE	70	11.704	12.237	34.017	1.00	29.61
ATOM	215	C	ILE	70	10.549	16.863	32.563	1.00	40.38
ATOM	216	O	ILE	70	10.937	16.993	31.402	1.00	43.43
ATOM	217	N	GLY	71	9.405	17.371	33.027	1.00	44.94
ATOM	218	CA	GLY	71	8.537	18.208	32.223	1.00	47.46
ATOM	219	C	GLY	71	7.578	17.485	31.304	1.00	48.54
ATOM	220	O	GLY	71	7.887	16.401	30.815	1.00	47.51
ATOM	221	N	SER	72	6.400	18.091	31.127	1.00	51.97
ATOM	222	CA	SER	72	5.307	17.630	30.253	1.00	53.80
ATOM	223	CB	SER	72	5.136	16.113	30.276	1.00	52.09
ATOM	224	OG	SER	72	5.997	15.516	29.320	1.00	55.01
ATOM	225	C	SER	72	3.971	18.307	30.555	1.00	53.60
ATOM	226	O	SER	72	3.776	18.723	31.719	1.00	56.25
ATOM	227	CB	GLN	75	-2.575	15.033	30.778	1.00	26.20
ATOM	228	CG	GLN	75	-2.224	13.624	31.177	1.00	27.29
ATOM	229	CD	GLN	75	-3.442	12.728	31.172	1.00	31.62
ATOM	230	OE1	GLN	75	-3.558	11.818	30.342	1.00	36.78
ATOM	231	NE2	GLN	75	-4.381	13.001	32.083	1.00	31.34
ATOM	232	C	GLN	75	-1.319	16.062	32.660	1.00	27.21
ATOM	233	O	GLN	75	-2.275	16.251	33.425	1.00	31.31
ATOM	234	N	GLN	75	-0.228	15.740	30.395	1.00	24.95

FIG. 1E

ATOM	235	CA	GLN	75	-1.501	16.040	31.140	1.00	27.33
ATOM	236	N	GLY	76	-0.114	15.722	33.081	1.00	23.74
ATOM	237	CA	GLY	76	0.247	15.754	34.480	1.00	22.16
ATOM	238	C	GLY	76	1.684	16.234	34.382	1.00	26.62
ATOM	239	O	GLY	76	2.233	16.275	33.273	1.00	31.92
ATOM	240	N	ILE	77	2.294	16.662	35.482	1.00	20.67
ATOM	241	CA	ILE	77	3.679	17.096	35.390	1.00	16.35
ATOM	242	CB	ILE	77	4.019	18.301	36.308	1.00	19.61
ATOM	243	CG2	ILE	77	5.504	18.705	36.124	1.00	12.60
ATOM	244	CG1	ILE	77	3.160	19.521	35.953	1.00	17.46
ATOM	245	CD1	ILE	77	1.659	19.354	36.135	1.00	18.13
ATOM	246	C	ILE	77	4.453	15.843	35.762	1.00	14.34
ATOM	247	O	ILE	77	3.934	14.986	36.477	1.00	15.37
ATOM	248	N	VAL	78	5.645	15.678	35.203	1.00	13.70
ATOM	249	CA	VAL	78	6.446	14.487	35.472	1.00	13.92
ATOM	250	CB	VAL	78	6.613	13.639	34.176	1.00	13.49
ATOM	251	CG1	VAL	78	7.578	12.482	34.393	1.00	11.19
ATOM	252	CG2	VAL	78	5.249	13.122	33.730	1.00	6.97
ATOM	253	C	VAL	78	7.804	14.768	36.098	1.00	15.53
ATOM	254	O	VAL	78	8.587	15.567	35.577	1.00	16.48
ATOM	255	N	CYS	79	8.097	14.038	37.176	1.00	16.79
ATOM	256	CA	CYS	79	9.345	14.181	37.923	1.00	12.30
ATOM	257	CB	CYS	79	9.063	14.590	39.375	1.00	17.48
ATOM	258	SG	CYS	79	8.724	16.334	39.667	1.00	17.95
ATOM	259	C	CYS	79	10.189	12.915	37.951	1.00	7.69
ATOM	260	O	CYS	79	9.677	11.804	37.991	1.00	10.14
ATOM	261	N	ALA	80	11.496	13.113	37.907	1.00	4.10
ATOM	262	CA	ALA	80	12.462	12.040	37.970	1.00	13.15
ATOM	263	CB	ALA	80	13.731	12.446	37.236	1.00	12.16
ATOM	264	C	ALA	80	12.772	11.840	39.452	1.00	21.14
ATOM	265	O	ALA	80	13.532	12.617	40.038	1.00	26.46
ATOM	266	N	ALA	81	12.211	10.798	40.055	1.00	21.98
ATOM	267	CA	ALA	81	12.458	10.536	41.472	1.00	21.56
ATOM	268	CB	ALA	81	11.139	10.221	42.180	1.00	17.84
ATOM	269	C	ALA	81	13.462	9.411	41.703	1.00	19.64
ATOM	270	O	ALA	81	14.131	8.960	40.770	1.00	21.54
ATOM	271	N	TYR	82	13.609	9.029	42.972	1.00	20.19
ATOM	272	CA	TYR	82	14.474	7.929	43.381	1.00	20.94
ATOM	273	CB	TYR	82	15.831	8.409	43.892	1.00	21.43
ATOM	274	CG	TYR	82	16.599	7.311	44.604	1.00	25.93
ATOM	275	CD1	TYR	82	17.105	6.218	43.907	1.00	29.90
ATOM	276	CE1	TYR	82	17.756	5.178	44.573	1.00	30.94
ATOM	277	CD2	TYR	82	16.772	7.337	45.985	1.00	25.81
ATOM	278	CE2	TYR	82	17.420	6.303	46.653	1.00	23.76
ATOM	279	CZ	TYR	82	17.903	5.230	45.946	1.00	30.58
ATOM	280	OH	TYR	82	18.500	4.196	46.618	1.00	29.44
ATOM	281	C	TYR	82	13.758	7.163	44.480	1.00	20.67
ATOM	282	O	TYR	82	13.568	7.684	45.576	1.00	23.05
ATOM	283	N	ASP	83	13.371	5.927	44.183	1.00	17.38
ATOM	284	CA	ASP	83	12.667	5.098	45.145	1.00	15.03
ATOM	285	CB	ASP	83	11.861	4.034	44.434	1.00	14.45
ATOM	286	CG	ASP	83	10.693	3.567	45.247	1.00	17.56
ATOM	287	OD1	ASP	83	10.777	3.604	46.496	1.00	18.87
ATOM	288	OD2	ASP	83	9.681	3.177	44.632	1.00	22.51
ATOM	289	C	ASP	83	13.648	4.432	46.088	1.00	19.10
ATOM	290	O	ASP	83	14.315	3.470	45.710	1.00	19.53
ATOM	291	N	ALA	84	13.667	4.905	47.335	1.00	18.37
ATOM	292	CA	ALA	84	14.569	4.401	48.367	1.00	13.42
ATOM	293	CB	ALA	84	14.492	5.290	49.595	1.00	16.90

FIG. 1F

ATOM	294	C	ALA	84	14.264	2.967	48.737	1.00	7.60
ATOM	295	O	ALA	84	15.178	2.180	48.967	1.00	7.42
ATOM	296	N	VAL	85	12.983	2.622	48.754	1.00	2.00
ATOM	297	CA	VAL	85	12.557	1.270	49.086	1.00	11.88
ATOM	298	CB	VAL	85	11.023	1.208	49.289	1.00	15.00
ATOM	299	CG1	VAL	85	10.608	-0.176	49.738	1.00	18.62
ATOM	300	CG2	VAL	85	10.588	2.250	50.314	1.00	11.37
ATOM	301	C	VAL	85	12.979	0.217	48.042	1.00	15.24
ATOM	302	O	VAL	85	13.496	-0.845	48.391	1.00	17.38
ATOM	303	N	LEU	86	12.772	0.533	46.765	1.00	17.84
ATOM	304	CA	LEU	86	13.118	-0.369	45.664	1.00	13.79
ATOM	305	CB	LEU	86	12.144	-0.177	44.515	1.00	12.13
ATOM	306	CG	LEU	86	10.866	-1.006	44.534	1.00	12.71
ATOM	307	CD1	LEU	86	10.245	-1.065	45.909	1.00	16.53
ATOM	308	CD2	LEU	86	9.910	-0.409	43.536	1.00	14.81
ATOM	309	C	LEU	86	14.529	-0.191	45.129	1.00	17.04
ATOM	310	O	LEU	86	15.020	-1.035	44.382	1.00	21.60
ATOM	311	N	ASP	87	15.186	0.891	45.530	1.00	18.90
ATOM	312	CA	ASP	87	16.539	1.204	45.079	1.00	23.81
ATOM	313	CB	ASP	87	17.543	0.151	45.551	1.00	22.37
ATOM	314	CG	ASP	87	18.984	0.609	45.381	1.00	30.15
ATOM	315	OD1	ASP	87	19.271	1.797	45.637	1.00	29.63
ATOM	316	OD2	ASP	87	19.836	-0.212	44.981	1.00	35.59
ATOM	317	C	ASP	87	16.664	1.391	43.567	1.00	25.14
ATOM	318	O	ASP	87	17.634	0.937	42.948	1.00	28.93
ATOM	319	N	ARG	88	15.691	2.071	42.979	1.00	24.77
ATOM	320	CA	ARG	88	15.710	2.335	41.546	1.00	23.82
ATOM	321	CB	ARG	88	14.940	1.270	40.769	1.00	21.43
ATOM	322	CG	ARG	88	13.481	1.152	41.185	1.00	26.04
ATOM	323	CD	ARG	88	12.588	0.723	40.042	1.00	35.46
ATOM	324	NE	ARG	88	13.157	-0.353	39.224	1.00	43.22
ATOM	325	CZ	ARG	88	12.473	-1.048	38.314	1.00	43.53
ATOM	326	NH1	ARG	88	11.185	-0.796	38.104	1.00	42.29
ATOM	327	NH2	ARG	88	13.083	-1.977	37.583	1.00	47.38
ATOM	328	C	ARG	88	15.078	3.691	41.299	1.00	21.16
ATOM	329	O	ARG	88	14.143	4.080	41.995	1.00	19.00
ATOM	330	N	ASN	89	15.592	4.402	40.297	1.00	18.57
ATOM	331	CA	ASN	89	15.073	5.716	39.951	1.00	10.01
ATOM	332	CB	ASN	89	15.949	6.402	38.905	1.00	12.28
ATOM	333	CG	ASN	89	17.437	6.099	39.063	1.00	20.41
ATOM	334	OD1	ASN	89	17.838	4.942	39.186	1.00	31.61
ATOM	335	ND2	ASN	89	18.262	7.139	39.020	1.00	19.05
ATOM	336	C	ASN	89	13.716	5.447	39.344	1.00	4.86
ATOM	337	O	ASN	89	13.534	4.452	38.650	1.00	7.53
ATOM	338	N	VAL	90	12.740	6.277	39.675	1.00	5.33
ATOM	339	CA	VAL	90	11.399	6.127	39.128	1.00	2.00
ATOM	340	CB	VAL	90	10.408	5.600	40.186	1.00	4.37
ATOM	341	CG1	VAL	90	10.862	4.240	40.702	1.00	7.02
ATOM	342	CG2	VAL	90	10.254	6.597	41.321	1.00	6.06
ATOM	343	C	VAL	90	10.893	7.454	38.545	1.00	4.05
ATOM	344	O	VAL	90	11.662	8.397	38.347	1.00	5.57
ATOM	345	N	ALA	91	9.609	7.500	38.212	1.00	2.00
ATOM	346	CA	ALA	91	8.984	8.704	37.679	1.00	3.61
ATOM	347	CB	ALA	91	8.920	8.670	36.151	1.00	5.67
ATOM	348	C	ALA	91	7.589	8.771	38.270	1.00	10.32
ATOM	349	O	ALA	91	6.900	7.751	38.412	1.00	13.32
ATOM	350	N	ILE	92	7.193	9.976	38.657	1.00	12.22
ATOM	351	CA	ILE	92	5.889	10.198	39.257	1.00	13.29
ATOM	352	CB	ILE	92	6.063	10.804	40.697	1.00	15.08

FIG. 1G

ATOM	353	CG2	ILE	92	4.800	10.584	41.536	1.00	9.12
ATOM	354	CG1	ILE	92	7.269	10.161	41.400	1.00	14.98
ATOM	355	CD1	ILE	92	7.639	10.804	42.711	1.00	17.01
ATOM	356	C	ILE	92	5.133	11.181	38.368	1.00	12.70
ATOM	357	O	ILE	92	5.749	12.012	37.702	1.00	13.94
ATOM	358	N	LYS	93	3.811	11.055	38.323	1.00	10.80
ATOM	359	CA	LYS	93	2.993	11.962	37.534	1.00	12.68
ATOM	360	CB	LYS	93	2.523	11.301	36.238	1.00	18.72
ATOM	361	CG	LYS	93	1.678	12.217	35.356	1.00	26.15
ATOM	362	CD	LYS	93	1.476	11.675	33.953	1.00	33.36
ATOM	363	CE	LYS	93	0.568	10.453	33.920	1.00	38.49
ATOM	364	NZ	LYS	93	0.554	9.814	32.569	1.00	45.17
ATOM	365	C	LYS	93	1.800	12.403	38.364	1.00	12.16
ATOM	366	O	LYS	93	1.090	11.582	38.936	1.00	12.27
ATOM	367	N	LYS	94	1.566	13.705	38.415	1.00	12.37
ATOM	368	CA	LYS	94	0.467	14.226	39.214	1.00	13.50
ATOM	369	CB	LYS	94	0.933	15.404	40.080	1.00	11.86
ATOM	370	CG	LYS	94	-0.094	15.759	41.148	1.00	14.06
ATOM	371	CD	LYS	94	-0.275	17.250	41.372	1.00	12.12
ATOM	372	CE	LYS	94	0.889	17.881	42.073	1.00	15.03
ATOM	373	NZ	LYS	94	0.418	19.124	42.737	1.00	21.64
ATOM	374	C	LYS	94	-0.760	14.657	38.442	1.00	13.08
ATOM	375	O	LYS	94	-0.704	15.562	37.616	1.00	18.01
ATOM	376	N	LEU	95	-1.877	14.017	38.741	1.00	14.19
ATOM	377	CA	LEU	95	-3.142	14.351	38.120	1.00	13.05
ATOM	378	CB	LEU	95	-3.913	13.090	37.718	1.00	17.09
ATOM	379	CG	LEU	95	-3.643	12.386	36.391	1.00	15.05
ATOM	380	CD1	LEU	95	-2.201	11.920	36.310	1.00	15.02
ATOM	381	CD2	LEU	95	-4.602	11.207	36.267	1.00	17.68
ATOM	382	C	LEU	95	-3.969	15.093	39.153	1.00	17.18
ATOM	383	O	LEU	95	-4.535	14.480	40.049	1.00	18.32
ATOM	384	N	SER	96	-4.030	16.412	39.035	1.00	17.90
ATOM	385	CA	SER	96	-4.814	17.212	39.958	1.00	16.67
ATOM	386	CB	SER	96	-4.283	18.645	40.036	1.00	20.30
ATOM	387	OG	SER	96	-2.903	18.681	40.351	1.00	30.22
ATOM	388	C	SER	96	-6.268	17.242	39.518	1.00	16.31
ATOM	389	O	SER	96	-6.567	17.551	38.369	1.00	23.36
ATOM	390	N	ARG	97	-7.164	16.915	40.443	1.00	13.24
ATOM	391	CA	ARG	97	-8.607	16.924	40.198	1.00	14.86
ATOM	392	CB	ARG	97	-9.164	18.349	40.326	1.00	17.53
ATOM	393	CG	ARG	97	-8.944	18.996	41.669	1.00	17.18
ATOM	394	CD	ARG	97	-9.733	20.285	41.788	1.00	19.58
ATOM	395	NE	ARG	97	-9.465	20.914	43.072	1.00	27.92
ATOM	396	CZ	ARG	97	-10.120	20.649	44.200	1.00	29.09
ATOM	397	NH1	ARG	97	-11.119	19.771	44.229	1.00	33.26
ATOM	398	NH2	ARG	97	-9.723	21.217	45.326	1.00	25.41
ATOM	399	C	ARG	97	-9.061	16.331	38.865	1.00	16.76
ATOM	400	O	ARG	97	-9.819	16.954	38.127	1.00	17.95
ATOM	401	N	PRO	98	-8.634	15.097	38.562	1.00	17.80
ATOM	402	CD	PRO	98	-7.815	14.196	39.385	1.00	18.27
ATOM	403	CA	PRO	98	-9.015	14.448	37.305	1.00	14.40
ATOM	404	CB	PRO	98	-8.280	13.110	37.378	1.00	14.74
ATOM	405	CG	PRO	98	-8.172	12.843	38.838	1.00	15.84
ATOM	406	C	PRO	98	-10.523	14.275	37.128	1.00	14.36
ATOM	407	O	PRO	98	-11.018	14.251	36.001	1.00	18.45
ATOM	408	N	PHE	99	-11.247	14.178	38.237	1.00	11.59
ATOM	409	CA	PHE	99	-12.702	14.005	38.240	1.00	8.51
ATOM	410	CB	PHE	99	-13.166	13.512	39.625	1.00	10.76
ATOM	411	CG	PHE	99	-12.577	14.301	40.775	1.00	11.82

FIG. 1H

ATOM	412	CD1	PHE	99	-11.334	13.954	41.297	1.00	9.19
ATOM	413	CD2	PHE	99	-13.211	15.456	41.248	1.00	11.64
ATOM	414	CE1	PHE	99	-10.718	14.753	42.255	1.00	10.55
ATOM	415	CE2	PHE	99	-12.604	16.266	42.210	1.00	3.04
ATOM	416	CZ	PHE	99	-11.354	15.918	42.711	1.00	3.99
ATOM	417	C	PHE	99	-13.479	15.272	37.864	1.00	9.70
ATOM	418	O	PHE	99	-14.710	15.223	37.780	1.00	4.45
ATOM	419	N	GLN	100	-12.785	16.395	37.643	1.00	14.64
ATOM	420	CA	GLN	100	-13.453	17.660	37.286	1.00	21.27
ATOM	421	CB	GLN	100	-12.672	18.874	37.810	1.00	21.59
ATOM	422	CG	GLN	100	-12.635	18.961	39.332	1.00	25.09
ATOM	423	CD	GLN	100	-13.299	20.216	39.918	1.00	29.38
ATOM	424	OE1	GLN	100	-12.865	20.716	40.963	1.00	26.88
ATOM	425	NE2	GLN	100	-14.380	20.695	39.285	1.00	28.47
ATOM	426	C	GLN	100	-13.798	17.854	35.808	1.00	23.90
ATOM	427	O	GLN	100	-14.617	18.721	35.468	1.00	24.03
ATOM	428	N	ASN	101	-13.181	17.054	34.942	1.00	25.19
ATOM	429	CA	ASN	101	-13.430	17.105	33.502	1.00	24.30
ATOM	430	CB	ASN	101	-12.143	17.447	32.743	1.00	28.04
ATOM	431	CG	ASN	101	-12.352	17.515	31.241	1.00	31.27
ATOM	432	OD1	ASN	101	-12.109	16.543	30.531	1.00	37.00
ATOM	433	ND2	ASN	101	-12.801	18.666	30.751	1.00	32.53
ATOM	434	C	ASN	101	-13.933	15.738	33.069	1.00	21.66
ATOM	435	O	ASN	101	-13.186	14.767	33.103	1.00	20.60
ATOM	436	N	GLN	102	-15.191	15.676	32.643	1.00	19.05
ATOM	437	CA	GLN	102	-15.824	14.430	32.210	1.00	24.39
ATOM	438	CB	GLN	102	-17.060	14.741	31.372	1.00	27.49
ATOM	439	CG	GLN	102	-17.874	13.518	31.001	1.00	36.15
ATOM	440	CD	GLN	102	-18.898	13.166	32.066	1.00	42.89
ATOM	441	OE1	GLN	102	-19.578	14.048	32.600	1.00	43.41
ATOM	442	NE2	GLN	102	-19.022	11.874	32.375	1.00	41.93
ATOM	443	C	GLN	102	-14.929	13.474	31.413	1.00	23.63
ATOM	444	O	GLN	102	-15.050	12.257	31.548	1.00	24.99
ATOM	445	N	THR	103	-14.066	14.029	30.562	1.00	20.69
ATOM	446	CA	THR	103	-13.158	13.246	29.730	1.00	17.84
ATOM	447	CB	THR	103	-12.702	14.052	28.504	1.00	17.02
ATOM	448	OG1	THR	103	-13.839	14.415	27.718	1.00	19.48
ATOM	449	CG2	THR	103	-11.724	13.253	27.665	1.00	11.85
ATOM	450	C	THR	103	-11.905	12.815	30.480	1.00	20.98
ATOM	451	O	THR	103	-11.425	11.691	30.306	1.00	24.66
ATOM	452	N	HIS	104	-11.328	13.744	31.242	1.00	20.55
ATOM	453	CA	HIS	104	-10.129	13.466	32.035	1.00	15.76
ATOM	454	CB	HIS	104	-9.617	14.751	32.678	1.00	15.65
ATOM	455	CG	HIS	104	-8.759	15.578	31.780	1.00	10.94
ATOM	456	CD2	HIS	104	-7.423	15.789	31.776	1.00	18.06
ATOM	457	ND1	HIS	104	-9.269	16.318	30.736	1.00	11.77
ATOM	458	CE1	HIS	104	-8.283	16.953	30.127	1.00	19.65
ATOM	459	NE2	HIS	104	-7.151	16.650	30.738	1.00	19.90
ATOM	460	C	HIS	104	-10.464	12.452	33.127	1.00	14.82
ATOM	461	O	HIS	104	-9.615	11.667	33.546	1.00	13.77
ATOM	462	N	ALA	105	-11.728	12.469	33.536	1.00	11.82
ATOM	463	CA	ALA	105	-12.252	11.602	34.565	1.00	8.37
ATOM	464	CB	ALA	105	-13.651	12.031	34.911	1.00	6.82
ATOM	465	C	ALA	105	-12.262	10.182	34.049	1.00	10.85
ATOM	466	O	ALA	105	-11.449	9.353	34.459	1.00	13.46
ATOM	467	N	LYS	106	-13.141	9.944	33.078	1.00	12.30
ATOM	468	CA	LYS	106	-13.322	8.647	32.445	1.00	10.14
ATOM	469	CB	LYS	106	-14.186	8.822	31.197	1.00	22.07
ATOM	470	CG	LYS	106	-14.983	7.587	30.792	1.00	32.05

FIG. 1I

ATOM	471	CD	LYS	106	-15.989	7.883	29.669	1.00	38.01
ATOM	472	CE	LYS	106	-17.129	8.834	30.090	1.00	38.61
ATOM	473	NZ	LYS	106	-16.846	10.302	29.933	1.00	32.07
ATOM	474	C	LYS	106	-11.959	8.082	32.080	1.00	7.28
ATOM	475	O	LYS	106	-11.645	6.933	32.376	1.00	8.85
ATOM	476	N	ARG	107	-11.117	8.938	31.521	1.00	7.12
ATOM	477	CA	ARG	107	-9.782	8.547	31.126	1.00	7.00
ATOM	478	CB	ARG	107	-9.051	9.740	30.503	1.00	6.80
ATOM	479	CG	ARG	107	-7.647	9.444	30.016	1.00	12.16
ATOM	480	CD	ARG	107	-7.115	10.583	29.136	1.00	19.65
ATOM	481	NE	ARG	107	-5.842	10.259	28.479	1.00	28.47
ATOM	482	CZ	ARG	107	-5.717	9.538	27.365	1.00	23.50
ATOM	483	NH1	ARG	107	-6.790	9.047	26.753	1.00	23.94
ATOM	484	NH2	ARG	107	-4.513	9.320	26.852	1.00	24.62
ATOM	485	C	ARG	107	-9.002	7.984	32.300	1.00	6.34
ATOM	486	O	ARG	107	-8.558	6.850	32.232	1.00	12.54
ATOM	487	N	ALA	108	-8.905	8.745	33.393	1.00	13.11
ATOM	488	CA	ALA	108	-8.160	8.341	34.600	1.00	12.23
ATOM	489	CB	ALA	108	-8.183	9.452	35.612	1.00	16.56
ATOM	490	C	ALA	108	-8.605	7.040	35.266	1.00	9.84
ATOM	491	O	ALA	108	-7.775	6.231	35.687	1.00	9.07
ATOM	492	N	TYR	109	-9.911	6.854	35.394	1.00	7.50
ATOM	493	CA	TYR	109	-10.441	5.651	36.001	1.00	13.33
ATOM	494	CB	TYR	109	-11.959	5.744	36.083	1.00	19.72
ATOM	495	CG	TYR	109	-12.603	4.518	36.669	1.00	22.28
ATOM	496	CD1	TYR	109	-12.213	4.035	37.908	1.00	23.99
ATOM	497	CE1	TYR	109	-12.825	2.929	38.466	1.00	25.88
ATOM	498	CD2	TYR	109	-13.623	3.862	36.001	1.00	22.06
ATOM	499	CE2	TYR	109	-14.241	2.752	36.554	1.00	21.88
ATOM	500	CZ	TYR	109	-13.838	2.292	37.785	1.00	26.78
ATOM	501	OH	TYR	109	-14.460	1.200	38.341	1.00	33.91
ATOM	502	C	TYR	109	-10.064	4.446	35.157	1.00	17.09
ATOM	503	O	TYR	109	-9.470	3.485	35.642	1.00	18.57
ATOM	504	N	ARG	110	-10.389	4.550	33.874	1.00	19.91
ATOM	505	CA	ARG	110	-10.157	3.533	32.865	1.00	17.79
ATOM	506	CB	ARG	110	-10.568	4.125	31.511	1.00	29.51
ATOM	507	CG	ARG	110	-10.758	3.137	30.369	1.00	32.16
ATOM	508	CD	ARG	110	-11.271	3.829	29.095	1.00	29.67
ATOM	509	NE	ARG	110	-10.935	3.039	27.916	1.00	30.13
ATOM	510	CZ	ARG	110	-9.733	3.030	27.350	1.00	29.42
ATOM	511	NH1	ARG	110	-8.756	3.786	27.843	1.00	31.13
ATOM	512	NH2	ARG	110	-9.482	2.204	26.342	1.00	29.18
ATOM	513	C	ARG	110	-8.714	3.044	32.823	1.00	16.76
ATOM	514	O	ARG	110	-8.458	1.842	32.828	1.00	16.62
ATOM	515	N	GLU	111	-7.766	3.973	32.798	1.00	15.33
ATOM	516	CA	GLU	111	-6.353	3.616	32.735	1.00	17.28
ATOM	517	CB	GLU	111	-5.498	4.878	32.580	1.00	21.45
ATOM	518	CG	GLU	111	-6.046	5.932	31.598	1.00	20.21
ATOM	519	CD	GLU	111	-5.777	5.641	30.133	1.00	19.30
ATOM	520	OE1	GLU	111	-4.670	5.984	29.672	1.00	8.75
ATOM	521	OE2	GLU	111	-6.683	5.124	29.437	1.00	22.37
ATOM	522	C	GLU	111	-5.913	2.853	33.977	1.00	16.99
ATOM	523	O	GLU	111	-5.020	2.000	33.918	1.00	15.26
ATOM	524	N	LEU	112	-6.538	3.192	35.103	1.00	22.40
ATOM	525	CA	LEU	112	-6.264	2.583	36.409	1.00	16.54
ATOM	526	CB	LEU	112	-6.919	3.446	37.493	1.00	15.35
ATOM	527	CG	LEU	112	-6.096	3.943	38.692	1.00	18.09
ATOM	528	CD1	LEU	112	-4.658	4.299	38.299	1.00	7.17
ATOM	529	CD2	LEU	112	-6.815	5.140	39.307	1.00	14.16

FIG. 1J

ATOM	530	C	LEU	112	-6.819	1.151	36.435	1.00	12.99
ATOM	531	O	LEU	112	-6.126	0.199	36.801	1.00	6.73
ATOM	532	N	VAL	113	-8.048	1.006	35.965	1.00	6.24
ATOM	533	CA	VAL	113	-8.707	-0.275	35.893	1.00	6.98
ATOM	534	CB	VAL	113	-10.187	-0.076	35.500	1.00	7.10
ATOM	535	CG1	VAL	113	-10.870	-1.409	35.272	1.00	12.66
ATOM	536	CG2	VAL	113	-10.910	0.713	36.577	1.00	12.28
ATOM	537	C	VAL	113	-8.033	-1.212	34.874	1.00	11.22
ATOM	538	O	VAL	113	-7.904	-2.414	35.114	1.00	15.98
ATOM	539	N	LEU	114	-7.554	-0.646	33.770	1.00	14.36
ATOM	540	CA	LEU	114	-6.927	-1.423	32.707	1.00	16.13
ATOM	541	CB	LEU	114	-7.010	-0.679	31.375	1.00	15.67
ATOM	542	CG	LEU	114	-8.393	-0.629	30.753	1.00	12.06
ATOM	543	CD1	LEU	114	-8.282	0.021	29.404	1.00	17.14
ATOM	544	CD2	LEU	114	-8.937	-2.036	30.614	1.00	17.36
ATOM	545	C	LEU	114	-5.500	-1.846	32.931	1.00	16.07
ATOM	546	O	LEU	114	-4.999	-2.719	32.225	1.00	21.08
ATOM	547	N	MET	115	-4.836	-1.252	33.905	1.00	16.41
ATOM	548	CA	MET	115	-3.455	-1.617	34.149	1.00	16.95
ATOM	549	CB	MET	115	-2.727	-0.509	34.895	1.00	20.21
ATOM	550	CG	MET	115	-1.350	-0.250	34.333	1.00	19.72
ATOM	551	SD	MET	115	-0.698	1.312	34.874	1.00	28.78
ATOM	552	CE	MET	115	-1.885	2.433	34.130	1.00	25.09
ATOM	553	C	MET	115	-3.335	-2.950	34.871	1.00	16.08
ATOM	554	O	MET	115	-2.244	-3.499	34.991	1.00	18.48
ATOM	555	N	LYS	116	-4.472	-3.459	35.334	1.00	18.87
ATOM	556	CA	LYS	116	-4.542	-4.744	36.015	1.00	23.57
ATOM	557	CB	LYS	116	-5.706	-4.749	37.021	1.00	26.91
ATOM	558	CG	LYS	116	-5.551	-3.731	38.161	1.00	33.65
ATOM	559	CD	LYS	116	-6.631	-3.843	39.247	1.00	35.36
ATOM	560	CE	LYS	116	-7.921	-3.092	38.909	1.00	36.42
ATOM	561	NZ	LYS	116	-8.741	-3.743	37.845	1.00	37.10
ATOM	562	C	LYS	116	-4.767	-5.825	34.956	1.00	25.45
ATOM	563	O	LYS	116	-4.443	-6.995	35.162	1.00	24.99
ATOM	564	N	CYS	117	-5.306	-5.397	33.813	1.00	22.92
ATOM	565	CA	CYS	117	-5.613	-6.267	32.689	1.00	15.45
ATOM	566	CB	CYS	117	-6.767	-5.679	31.890	1.00	12.92
ATOM	567	SG	CYS	117	-8.238	-5.322	32.853	1.00	21.59
ATOM	568	C	CYS	117	-4.451	-6.493	31.732	1.00	15.36
ATOM	569	O	CYS	117	-4.565	-7.300	30.814	1.00	20.75
ATOM	570	N	VAL	118	-3.344	-5.784	31.929	1.00	17.19
ATOM	571	CA	VAL	118	-2.185	-5.916	31.041	1.00	19.32
ATOM	572	CB	VAL	118	-2.062	-4.670	30.111	1.00	18.65
ATOM	573	CG1	VAL	118	-0.804	-4.740	29.267	1.00	25.76
ATOM	574	CG2	VAL	118	-3.286	-4.556	29.217	1.00	16.20
ATOM	575	C	VAL	118	-0.841	-6.136	31.744	1.00	19.05
ATOM	576	O	VAL	118	-0.680	-5.816	32.917	1.00	22.85
ATOM	577	N	THR	119	0.108	-6.726	31.023	1.00	17.25
ATOM	578	CA	THR	119	1.444	-6.962	31.546	1.00	18.76
ATOM	579	CB	THR	119	1.429	-8.081	32.623	1.00	18.92
ATOM	580	OG1	THR	119	2.769	-8.438	32.995	1.00	6.16
ATOM	581	CG2	THR	119	0.670	-9.301	32.129	1.00	26.90
ATOM	582	C	THR	119	2.414	-7.273	30.406	1.00	19.69
ATOM	583	O	THR	119	2.474	-8.402	29.908	1.00	25.39
ATOM	584	N	HIS	120	3.170	-6.259	29.988	1.00	17.60
ATOM	585	CA	HIS	120	4.125	-6.423	28.888	1.00	8.64
ATOM	586	CB	HIS	120	3.359	-6.285	27.568	1.00	17.21
ATOM	587	CG	HIS	120	4.074	-6.841	26.371	1.00	16.80
ATOM	588	CD2	HIS	120	5.268	-6.531	25.816	1.00	19.94

FIG. 1K

ATOM	589	ND1	HIS	120	3.538	-7.834	25.585	1.00	14.74
ATOM	590	CE1	HIS	120	4.367	-8.115	24.598	1.00	13.09
ATOM	591	NE2	HIS	120	5.426	-7.338	24.717	1.00	15.49
ATOM	592	C	HIS	120	5.197	-5.346	28.996	1.00	2.84
ATOM	593	O	HIS	120	4.887	-4.197	29.245	1.00	2.73
ATOM	594	N	LYS	121	6.452	-5.709	28.750	1.00	2.00
ATOM	595	CA	LYS	121	7.568	-4.770	28.844	1.00	5.68
ATOM	596	CB	LYS	121	8.908	-5.490	28.616	1.00	6.54
ATOM	597	CG	LYS	121	9.144	-5.913	27.166	1.00	19.16
ATOM	598	CD	LYS	121	10.552	-6.453	26.901	1.00	25.40
ATOM	599	CE	LYS	121	11.608	-5.352	26.768	1.00	32.20
ATOM	600	NZ	LYS	121	12.953	-5.909	26.390	1.00	30.85
ATOM	601	C	LYS	121	7.477	-3.594	27.876	1.00	12.80
ATOM	602	O	LYS	121	8.339	-2.714	27.883	1.00	18.97
ATOM	603	N	ASN	122	6.483	-3.613	26.995	1.00	15.97
ATOM	604	CA	ASN	122	6.310	-2.529	26.036	1.00	15.61
ATOM	605	CB	ASN	122	6.308	-3.077	24.602	1.00	22.61
ATOM	606	CG	ASN	122	7.577	-3.861	24.264	1.00	20.48
ATOM	607	OD1	ASN	122	7.516	-5.032	23.900	1.00	26.08
ATOM	608	ND2	ASN	122	8.732	-3.218	24.413	1.00	20.44
ATOM	609	C	ASN	122	5.024	-1.787	26.362	1.00	12.94
ATOM	610	O	ASN	122	4.501	-1.023	25.554	1.00	13.23
ATOM	611	N	ILE	123	4.521	-2.034	27.561	1.00	8.08
ATOM	612	CA	ILE	123	3.325	-1.391	28.057	1.00	12.42
ATOM	613	CB	ILE	123	2.107	-2.339	28.020	1.00	11.96
ATOM	614	CG2	ILE	123	0.891	-1.662	28.611	1.00	7.57
ATOM	615	CG1	ILE	123	1.805	-2.736	26.573	1.00	17.32
ATOM	616	CD1	ILE	123	1.385	-1.579	25.677	1.00	15.53
ATOM	617	C	ILE	123	3.623	-0.915	29.484	1.00	18.69
ATOM	618	O	ILE	123	4.462	-1.480	30.183	1.00	21.74
ATOM	619	N	ILE	124	2.966	0.164	29.895	1.00	22.62
ATOM	620	CA	ILE	124	3.174	0.763	31.208	1.00	20.00
ATOM	621	CB	ILE	124	2.404	2.106	31.338	1.00	16.67
ATOM	622	CG2	ILE	124	0.902	1.890	31.120	1.00	15.34
ATOM	623	CG1	ILE	124	2.694	2.740	32.699	1.00	7.20
ATOM	624	CD1	ILE	124	2.108	4.106	32.873	1.00	11.63
ATOM	625	C	ILE	124	2.853	-0.104	32.423	1.00	20.91
ATOM	626	O	ILE	124	1.765	-0.685	32.527	1.00	19.21
ATOM	627	N	SER	125	3.819	-0.170	33.339	1.00	20.40
ATOM	628	CA	SER	125	3.680	-0.917	34.594	1.00	19.59
ATOM	629	CB	SER	125	4.782	-1.974	34.750	1.00	23.73
ATOM	630	OG	SER	125	6.055	-1.375	34.987	1.00	31.90
ATOM	631	C	SER	125	3.794	0.086	35.743	1.00	13.73
ATOM	632	O	SER	125	4.892	0.559	36.075	1.00	4.90
ATOM	633	N	LEU	126	2.645	0.438	36.301	1.00	6.91
ATOM	634	CA	LEU	126	2.578	1.368	37.409	1.00	7.11
ATOM	635	CB	LEU	126	1.128	1.807	37.607	1.00	2.00
ATOM	636	CG	LEU	126	0.801	3.295	37.543	1.00	2.00
ATOM	637	CD1	LEU	126	1.449	3.953	36.336	1.00	2.00
ATOM	638	CD2	LEU	126	-0.704	3.451	37.508	1.00	2.04
ATOM	639	C	LEU	126	3.108	0.694	38.689	1.00	10.24
ATOM	640	O	LEU	126	2.604	-0.345	39.112	1.00	10.17
ATOM	641	N	LEU	127	4.157	1.268	39.268	1.00	11.75
ATOM	642	CA	LEU	127	4.751	0.744	40.491	1.00	10.20
ATOM	643	CB	LEU	127	6.199	1.219	40.622	1.00	3.15
ATOM	644	CG	LEU	127	7.253	0.763	39.619	1.00	7.77
ATOM	645	CD1	LEU	127	8.601	1.294	40.092	1.00	2.00
ATOM	646	CD2	LEU	127	7.278	-0.766	39.527	1.00	18.28
ATOM	647	C	LEU	127	3.995	1.145	41.770	1.00	12.88

FIG. 1L

ATOM	648	O	LEU	127	4.147	0.488	42.809	1.00	15.93
ATOM	649	N	ASN	128	3.192	2.209	41.704	1.00	14.08
ATOM	650	CA	ASN	128	2.460	2.679	42.883	1.00	14.71
ATOM	651	CB	ASN	128	3.473	3.186	43.923	1.00	17.09
ATOM	652	CG	ASN	128	2.868	3.398	45.299	1.00	18.33
ATOM	653	OD1	ASN	128	1.686	3.131	45.530	1.00	18.44
ATOM	654	ND2	ASN	128	3.686	3.875	46.228	1.00	15.54
ATOM	655	C	ASN	128	1.482	3.800	42.523	1.00	13.51
ATOM	656	O	ASN	128	1.805	4.674	41.735	1.00	17.61
ATOM	657	N	VAL	129	0.306	3.769	43.136	1.00	12.90
ATOM	658	CA	VAL	129	-0.753	4.754	42.935	1.00	15.50
ATOM	659	CB	VAL	129	-2.024	4.065	42.385	1.00	16.54
ATOM	660	CG1	VAL	129	-3.127	5.066	42.150	1.00	14.67
ATOM	661	CG2	VAL	129	-1.703	3.312	41.127	1.00	21.62
ATOM	662	C	VAL	129	-1.091	5.342	44.311	1.00	20.34
ATOM	663	O	VAL	129	-1.519	4.607	45.206	1.00	22.82
ATOM	664	N	PHE	130	-0.928	6.653	44.494	1.00	22.42
ATOM	665	CA	PHE	130	-1.223	7.241	45.801	1.00	17.23
ATOM	666	CB	PHE	130	-0.026	7.082	46.727	1.00	9.18
ATOM	667	CG	PHE	130	1.126	7.968	46.380	1.00	3.29
ATOM	668	CD1	PHE	130	2.221	7.451	45.710	1.00	3.28
ATOM	669	CD2	PHE	130	1.129	9.309	46.753	1.00	2.00
ATOM	670	CE1	PHE	130	3.304	8.250	45.409	1.00	6.45
ATOM	671	CE2	PHE	130	2.201	10.125	46.461	1.00	2.00
ATOM	672	CZ	PHE	130	3.295	9.602	45.785	1.00	6.75
ATOM	673	C	PHE	130	-1.707	8.682	45.868	1.00	20.03
ATOM	674	O	PHE	130	-1.308	9.537	45.082	1.00	23.64
ATOM	675	N	THR	131	-2.511	8.949	46.892	1.00	20.98
ATOM	676	CA	THR	131	-3.068	10.269	47.129	1.00	16.85
ATOM	677	CB	THR	131	-4.611	10.245	47.082	1.00	11.46
ATOM	678	OG1	THR	131	-5.132	11.530	47.426	1.00	11.14
ATOM	679	CG2	THR	131	-5.163	9.211	48.031	1.00	7.42
ATOM	680	C	THR	131	-2.637	10.770	48.498	1.00	20.65
ATOM	681	O	THR	131	-2.667	10.026	49.474	1.00	25.07
ATOM	682	N	PRO	132	-2.151	12.016	48.569	1.00	21.95
ATOM	683	CD	PRO	132	-1.729	12.903	47.472	1.00	22.01
ATOM	684	CA	PRO	132	-1.733	12.554	49.868	1.00	20.75
ATOM	685	CB	PRO	132	-0.821	13.714	49.475	1.00	18.92
ATOM	686	CG	PRO	132	-1.429	14.194	48.195	1.00	22.75
ATOM	687	C	PRO	132	-2.944	12.996	50.709	1.00	19.68
ATOM	688	O	PRO	132	-2.797	13.419	51.852	1.00	24.00
ATOM	689	N	GLN	133	-4.142	12.878	50.146	1.00	17.03
ATOM	690	CA	GLN	133	-5.354	13.253	50.853	1.00	17.14
ATOM	691	CB	GLN	133	-6.425	13.764	49.892	1.00	16.91
ATOM	692	CG	GLN	133	-6.158	15.188	49.391	1.00	10.35
ATOM	693	CD	GLN	133	-5.370	15.225	48.102	1.00	13.14
ATOM	694	OE1	GLN	133	-5.778	14.646	47.112	1.00	3.25
ATOM	695	NE2	GLN	133	-4.239	15.913	48.108	1.00	10.03
ATOM	696	C	GLN	133	-5.864	12.064	51.657	1.00	21.25
ATOM	697	O	GLN	133	-5.723	10.910	51.239	1.00	22.26
ATOM	698	N	LYS	134	-6.449	12.353	52.815	1.00	22.44
ATOM	699	CA	LYS	134	-6.939	11.318	53.709	1.00	25.31
ATOM	700	CB	LYS	134	-6.562	11.671	55.156	1.00	27.68
ATOM	701	CG	LYS	134	-5.241	11.048	55.621	1.00	33.88
ATOM	702	CD	LYS	134	-4.014	11.475	54.805	1.00	33.67
ATOM	703	CE	LYS	134	-3.590	12.911	55.101	1.00	36.64
ATOM	704	NZ	LYS	134	-2.188	13.180	54.640	1.00	33.55
ATOM	705	C	LYS	134	-8.405	10.907	53.615	1.00	26.52
ATOM	706	O	LYS	134	-8.770	9.832	54.092	1.00	25.08

FIG. 1M

ATOM	707	N	THR	135	-9.252	11.755	53.042	1.00	27.26
ATOM	708	CA	THR	135	-10.666	11.416	52.896	1.00	29.66
ATOM	709	CB	THR	135	-11.543	12.164	53.913	1.00	31.92
ATOM	710	OG1	THR	135	-11.281	13.570	53.829	1.00	37.53
ATOM	711	CG2	THR	135	-11.257	11.676	55.327	1.00	34.45
ATOM	712	C	THR	135	-11.214	11.685	51.499	1.00	30.80
ATOM	713	O	THR	135	-10.553	12.299	50.657	1.00	29.91
ATOM	714	N	LEU	136	-12.446	11.235	51.272	1.00	31.35
ATOM	715	CA	LEU	136	-13.120	11.414	49.994	1.00	30.05
ATOM	716	CB	LEU	136	-14.418	10.611	49.955	1.00	25.71
ATOM	717	CG	LEU	136	-15.412	10.924	48.833	1.00	21.56
ATOM	718	CD1	LEU	136	-14.746	10.754	47.477	1.00	20.38
ATOM	719	CD2	LEU	136	-16.627	10.026	48.961	1.00	19.40
ATOM	720	C	LEU	136	-13.402	12.883	49.707	1.00	33.09
ATOM	721	O	LEU	136	-13.129	13.352	48.607	1.00	34.24
ATOM	722	N	GLU	137	-13.943	13.603	50.692	1.00	34.66
ATOM	723	CA	GLU	137	-14.244	15.019	50.500	1.00	36.88
ATOM	724	CB	GLU	137	-15.090	15.597	51.651	1.00	40.97
ATOM	725	CG	GLU	137	-14.366	15.793	52.994	1.00	45.75
ATOM	726	CD	GLU	137	-14.984	16.907	53.855	1.00	49.12
ATOM	727	OE1	GLU	137	-14.225	17.783	54.330	1.00	48.83
ATOM	728	OE2	GLU	137	-16.221	16.911	54.055	1.00	46.20
ATOM	729	C	GLU	137	-12.963	15.818	50.338	1.00	34.88
ATOM	730	O	GLU	137	-12.927	16.808	49.613	1.00	37.49
ATOM	731	N	GLU	138	-11.904	15.372	50.996	1.00	32.51
ATOM	732	CA	GLU	138	-10.631	16.059	50.920	1.00	33.95
ATOM	733	CB	GLU	138	-9.824	15.785	52.190	1.00	35.96
ATOM	734	CG	GLU	138	-8.508	16.532	52.268	1.00	38.62
ATOM	735	CD	GLU	138	-7.437	15.739	53.002	1.00	44.42
ATOM	736	OE1	GLU	138	-7.798	14.832	53.792	1.00	47.64
ATOM	737	OE2	GLU	138	-6.235	16.014	52.775	1.00	38.08
ATOM	738	C	GLU	138	-9.827	15.665	49.675	1.00	34.17
ATOM	739	O	GLU	138	-8.968	16.433	49.233	1.00	35.17
ATOM	740	N	PHE	139	-10.116	14.482	49.123	1.00	29.77
ATOM	741	CA	PHE	139	-9.452	13.934	47.935	1.00	23.01
ATOM	742	CB	PHE	139	-10.202	12.694	47.459	1.00	17.20
ATOM	743	CG	PHE	139	-9.651	12.103	46.186	1.00	12.63
ATOM	744	CD1	PHE	139	-8.285	11.903	46.033	1.00	10.00
ATOM	745	CD2	PHE	139	-10.500	11.781	45.128	1.00	7.51
ATOM	746	CE1	PHE	139	-7.768	11.406	44.848	1.00	4.34
ATOM	747	CE2	PHE	139	-9.999	11.286	43.944	1.00	4.17
ATOM	748	CZ	PHE	139	-8.627	11.096	43.799	1.00	2.93
ATOM	749	C	PHE	139	-9.359	14.946	46.792	1.00	23.97
ATOM	750	O	PHE	139	-10.377	15.493	46.355	1.00	25.86
ATOM	751	N	GLN	140	-8.160	15.122	46.247	1.00	21.95
ATOM	752	CA	GLN	140	-7.928	16.114	45.202	1.00	23.71
ATOM	753	CB	GLN	140	-7.313	17.340	45.874	1.00	25.69
ATOM	754	CG	GLN	140	-6.997	18.504	44.998	1.00	33.16
ATOM	755	CD	GLN	140	-6.506	19.667	45.824	1.00	36.46
ATOM	756	OE1	GLN	140	-7.130	20.722	45.861	1.00	40.80
ATOM	757	NE2	GLN	140	-5.402	19.464	46.533	1.00	36.20
ATOM	758	C	GLN	140	-7.035	15.631	44.052	1.00	22.46
ATOM	759	O	GLN	140	-7.459	15.619	42.898	1.00	24.38
ATOM	760	N	ASP	141	-5.806	15.244	44.383	1.00	19.44
ATOM	761	CA	ASP	141	-4.828	14.784	43.411	1.00	13.47
ATOM	762	CB	ASP	141	-3.531	15.551	43.626	1.00	13.18
ATOM	763	CG	ASP	141	-3.771	16.999	43.954	1.00	17.70
ATOM	764	OD1	ASP	141	-3.325	17.455	45.025	1.00	18.62
ATOM	765	OD2	ASP	141	-4.451	17.685	43.166	1.00	22.49

FIG. 1N

ATOM	766	C	ASP	141	-4.529	13.290	43.472	1.00	15.68
ATOM	767	O	ASP	141	-4.865	12.607	44.441	1.00	15.84
ATOM	768	N	VAL	142	-3.912	12.785	42.406	1.00	17.48
ATOM	769	CA	VAL	142	-3.516	11.379	42.296	1.00	10.30
ATOM	770	CB	VAL	142	-4.422	10.604	41.327	1.00	6.58
ATOM	771	CG1	VAL	142	-3.933	9.181	41.198	1.00	5.29
ATOM	772	CG2	VAL	142	-5.873	10.648	41.798	1.00	6.09
ATOM	773	C	VAL	142	-2.095	11.318	41.748	1.00	9.87
ATOM	774	O	VAL	142	-1.741	12.046	40.825	1.00	14.44
ATOM	775	N	TYR	143	-1.260	10.487	42.345	1.00	7.25
ATOM	776	CA	TYR	143	0.109	10.351	41.873	1.00	8.20
ATOM	777	CB	TYR	143	1.114	10.602	42.996	1.00	7.96
ATOM	778	CG	TYR	143	1.198	12.041	43.452	1.00	9.31
ATOM	779	CD1	TYR	143	0.144	12.645	44.136	1.00	10.72
ATOM	780	CE1	TYR	143	0.216	13.987	44.546	1.00	14.58
ATOM	781	CD2	TYR	143	2.332	12.809	43.193	1.00	7.27
ATOM	782	CE2	TYR	143	2.413	14.138	43.599	1.00	9.99
ATOM	783	CZ	TYR	143	1.352	14.725	44.273	1.00	16.33
ATOM	784	OH	TYR	143	1.442	16.047	44.664	1.00	17.53
ATOM	785	C	TYR	143	0.249	8.932	41.335	1.00	12.96
ATOM	786	O	TYR	143	-0.321	7.989	41.897	1.00	15.01
ATOM	787	N	LEU	144	0.916	8.807	40.188	1.00	14.02
ATOM	788	CA	LEU	144	1.143	7.520	39.530	1.00	6.63
ATOM	789	CB	LEU	144	0.498	7.521	38.147	1.00	3.96
ATOM	790	CG	LEU	144	-0.972	7.927	38.041	1.00	7.52
ATOM	791	CD1	LEU	144	-1.349	8.089	36.575	1.00	4.64
ATOM	792	CD2	LEU	144	-1.879	6.901	38.714	1.00	7.15
ATOM	793	C	LEU	144	2.649	7.352	39.384	1.00	8.82
ATOM	794	O	LEU	144	3.327	8.239	38.857	1.00	8.56
ATOM	795	N	VAL	145	3.175	6.229	39.869	1.00	9.85
ATOM	796	CA	VAL	145	4.614	5.965	39.804	1.00	10.26
ATOM	797	CB	VAL	145	5.178	5.548	41.177	1.00	4.81
ATOM	798	CG1	VAL	145	6.701	5.576	41.147	1.00	2.00
ATOM	799	CG2	VAL	145	4.633	6.460	42.256	1.00	8.68
ATOM	800	C	VAL	145	4.896	4.889	38.769	1.00	10.28
ATOM	801	O	VAL	145	4.085	3.987	38.566	1.00	14.74
ATOM	802	N	MET	146	6.068	4.958	38.150	1.00	12.27
ATOM	803	CA	MET	146	6.443	4.025	37.085	1.00	13.67
ATOM	804	CB	MET	146	5.900	4.589	35.766	1.00	19.39
ATOM	805	CG	MET	146	5.719	3.620	34.624	1.00	28.14
ATOM	806	SD	MET	146	5.591	4.490	33.031	1.00	15.16
ATOM	807	CE	MET	146	7.177	4.095	32.403	1.00	11.15
ATOM	808	C	MET	146	7.963	3.989	37.013	1.00	11.41
ATOM	809	O	MET	146	8.638	4.765	37.681	1.00	14.24
ATOM	810	N	GLU	147	8.510	3.101	36.194	1.00	12.24
ATOM	811	CA	GLU	147	9.958	3.026	36.057	1.00	10.39
ATOM	812	CB	GLU	147	10.359	1.764	35.301	1.00	13.37
ATOM	813	CG	GLU	147	11.869	1.594	35.228	1.00	20.29
ATOM	814	CD	GLU	147	12.306	0.436	34.356	1.00	20.99
ATOM	815	OE1	GLU	147	11.442	-0.188	33.700	1.00	21.78
ATOM	816	OE2	GLU	147	13.522	0.154	34.333	1.00	24.35
ATOM	817	C	GLU	147	10.446	4.260	35.296	1.00	7.60
ATOM	818	O	GLU	147	9.725	4.810	34.471	1.00	8.87
ATOM	819	N	LEU	148	11.678	4.673	35.552	1.00	9.62
ATOM	820	CA	LEU	148	12.229	5.851	34.897	1.00	9.07
ATOM	821	CB	LEU	148	13.273	6.527	35.794	1.00	9.50
ATOM	822	CG	LEU	148	13.777	7.907	35.349	1.00	2.00
ATOM	823	CD1	LEU	148	12.635	8.897	35.386	1.00	2.00
ATOM	824	CD2	LEU	148	14.917	8.373	36.224	1.00	2.00

FIG. 10

ATOM	825	C	LEU	148	12.836	5.617	33.521	1.00	14.45
ATOM	826	O	LEU	148	13.896	4.986	33.382	1.00	10.38
ATOM	827	N	MET	149	12.190	6.207	32.516	1.00	20.38
ATOM	828	CA	MET	149	12.637	6.128	31.124	1.00	18.31
ATOM	829	CB	MET	149	11.440	5.978	30.181	1.00	15.17
ATOM	830	CG	MET	149	10.546	4.739	30.472	1.00	13.81
ATOM	831	SD	MET	149	11.392	3.117	30.550	1.00	14.34
ATOM	832	CE	MET	149	11.336	2.605	28.796	1.00	7.98
ATOM	833	C	MET	149	13.435	7.393	30.817	1.00	17.37
ATOM	834	O	MET	149	13.161	8.458	31.382	1.00	14.19
ATOM	835	N	ASP	150	14.432	7.255	29.946	1.00	18.71
ATOM	836	CA	ASP	150	15.335	8.347	29.569	1.00	19.67
ATOM	837	CB	ASP	150	16.615	7.768	28.963	1.00	20.46
ATOM	838	CG	ASP	150	17.313	6.786	29.887	1.00	25.54
ATOM	839	OD1	ASP	150	16.738	6.394	30.928	1.00	33.84
ATOM	840	OD2	ASP	150	18.455	6.398	29.572	1.00	29.63
ATOM	841	C	ASP	150	14.823	9.462	28.659	1.00	19.58
ATOM	842	O	ASP	150	15.312	10.595	28.742	1.00	19.97
ATOM	843	N	ALA	151	13.893	9.144	27.761	1.00	16.48
ATOM	844	CA	ALA	151	13.347	10.151	26.844	1.00	12.89
ATOM	845	CB	ALA	151	14.307	10.386	25.668	1.00	13.41
ATOM	846	C	ALA	151	12.017	9.681	26.321	1.00	9.93
ATOM	847	O	ALA	151	11.587	8.580	26.649	1.00	12.65
ATOM	848	N	ASN	152	11.309	10.555	25.615	1.00	6.98
ATOM	849	CA	ASN	152	10.053	10.144	25.019	1.00	14.22
ATOM	850	CB	ASN	152	8.881	11.095	25.325	1.00	15.50
ATOM	851	CG	ASN	152	9.113	12.510	24.852	1.00	22.15
ATOM	852	OD1	ASN	152	8.257	13.092	24.180	1.00	22.15
ATOM	853	ND2	ASN	152	10.232	13.098	25.253	1.00	33.84
ATOM	854	C	ASN	152	10.349	10.018	23.535	1.00	19.02
ATOM	855	O	ASN	152	11.479	10.301	23.114	1.00	15.48
ATOM	856	N	LEU	153	9.365	9.577	22.750	1.00	19.93
ATOM	857	CA	LEU	153	9.561	9.371	21.316	1.00	15.53
ATOM	858	CB	LEU	153	8.370	8.655	20.694	1.00	11.21
ATOM	859	CG	LEU	153	8.669	7.298	20.059	1.00	8.57
ATOM	860	CD1	LEU	153	7.553	7.003	19.109	1.00	3.71
ATOM	861	CD2	LEU	153	10.003	7.285	19.322	1.00	6.14
ATOM	862	C	LEU	153	9.885	10.622	20.519	1.00	15.22
ATOM	863	O	LEU	153	10.859	10.635	19.777	1.00	13.43
ATOM	864	N	CYS	154	9.107	11.684	20.714	1.00	15.83
ATOM	865	CA	CYS	154	9.311	12.947	20.005	1.00	13.76
ATOM	866	CB	CYS	154	8.434	14.036	20.617	1.00	11.00
ATOM	867	SG	CYS	154	6.668	13.722	20.491	1.00	25.02
ATOM	868	C	CYS	154	10.771	13.407	20.011	1.00	11.62
ATOM	869	O	CYS	154	11.220	14.080	19.085	1.00	16.82
ATOM	870	N	GLN	155	11.515	13.010	21.037	1.00	13.05
ATOM	871	CA	GLN	155	12.916	13.386	21.168	1.00	16.63
ATOM	872	CB	GLN	155	13.311	13.454	22.652	1.00	20.85
ATOM	873	CG	GLN	155	13.089	14.823	23.291	1.00	29.75
ATOM	874	CD	GLN	155	11.746	15.429	22.921	1.00	38.41
ATOM	875	OE1	GLN	155	10.697	14.911	23.299	1.00	44.89
ATOM	876	NE2	GLN	155	11.774	16.516	22.147	1.00	43.08
ATOM	877	C	GLN	155	13.823	12.436	20.415	1.00	15.29
ATOM	878	O	GLN	155	14.937	12.794	20.036	1.00	14.99
ATOM	879	N	VAL	156	13.324	11.227	20.191	1.00	14.81
ATOM	880	CA	VAL	156	14.056	10.194	19.475	1.00	14.38
ATOM	881	CB	VAL	156	13.539	8.759	19.853	1.00	12.39
ATOM	882	CG1	VAL	156	14.570	7.709	19.506	1.00	13.35
ATOM	883	CG2	VAL	156	13.224	8.670	21.319	1.00	14.14

FIG. 1P

ATOM	884	C	VAL	156	13.833	10.457	17.977	1.00	10.81
ATOM	885	O	VAL	156	14.767	10.403	17.179	1.00	10.61
ATOM	886	N	ILE	157	12.607	10.838	17.628	1.00	6.45
ATOM	887	CA	ILE	157	12.221	11.141	16.260	1.00	8.99
ATOM	888	CB	ILE	157	10.785	11.690	16.217	1.00	2.57
ATOM	889	CG2	ILE	157	10.543	12.480	14.940	1.00	2.00
ATOM	890	CG1	ILE	157	9.795	10.541	16.387	1.00	2.00
ATOM	891	CD1	ILE	157	8.334	10.969	16.410	1.00	2.00
ATOM	892	C	ILE	157	13.151	12.169	15.629	1.00	16.39
ATOM	893	O	ILE	157	13.500	12.066	14.451	1.00	22.03
ATOM	894	N	GLN	158	13.563	13.158	16.411	1.00	16.88
ATOM	895	CA	GLN	158	14.439	14.183	15.882	1.00	19.76
ATOM	896	CB	GLN	158	14.283	15.487	16.667	1.00	24.43
ATOM	897	CG	GLN	158	13.262	16.468	16.064	1.00	29.67
ATOM	898	CD	GLN	158	13.670	17.030	14.692	1.00	33.29
ATOM	899	OE1	GLN	158	14.844	16.990	14.293	1.00	32.74
ATOM	900	NE2	GLN	158	12.691	17.568	13.971	1.00	38.14
ATOM	901	C	GLN	158	15.898	13.787	15.773	1.00	21.28
ATOM	902	O	GLN	158	16.672	14.471	15.100	1.00	23.06
ATOM	903	N	MET	159	16.288	12.688	16.408	1.00	23.90
ATOM	904	CA	MET	159	17.679	12.256	16.333	1.00	27.52
ATOM	905	CB	MET	159	18.105	11.504	17.594	1.00	26.97
ATOM	906	CG	MET	159	17.551	10.111	17.752	1.00	28.99
ATOM	907	SD	MET	159	17.963	9.398	19.365	1.00	33.77
ATOM	908	CE	MET	159	19.687	8.923	19.107	1.00	25.01
ATOM	909	C	MET	159	17.883	11.410	15.089	1.00	29.07
ATOM	910	O	MET	159	16.944	10.796	14.592	1.00	26.59
ATOM	911	N	GLU	160	19.096	11.440	14.549	1.00	33.57
ATOM	912	CA	GLU	160	19.416	10.686	13.344	1.00	37.97
ATOM	913	CB	GLU	160	20.781	11.117	12.803	1.00	43.50
ATOM	914	CG	GLU	160	21.038	10.753	11.353	1.00	48.38
ATOM	915	CD	GLU	160	22.314	11.387	10.826	1.00	54.65
ATOM	916	OE1	GLU	160	22.292	12.602	10.523	1.00	57.49
ATOM	917	OE2	GLU	160	23.340	10.678	10.726	1.00	58.34
ATOM	918	C	GLU	160	19.396	9.191	13.649	1.00	40.57
ATOM	919	O	GLU	160	20.360	8.622	14.180	1.00	41.54
ATOM	920	N	LEU	161	18.255	8.578	13.358	1.00	40.99
ATOM	921	CA	LEU	161	18.055	7.156	13.595	1.00	38.14
ATOM	922	CB	LEU	161	16.623	6.870	14.057	1.00	32.66
ATOM	923	CG	LEU	161	16.120	7.358	15.409	1.00	27.51
ATOM	924	CD1	LEU	161	14.610	7.176	15.456	1.00	21.09
ATOM	925	CD2	LEU	161	16.808	6.606	16.542	1.00	18.19
ATOM	926	C	LEU	161	18.320	6.326	12.352	1.00	37.38
ATOM	927	O	LEU	161	17.863	6.652	11.252	1.00	38.37
ATOM	928	N	ASP	162	19.081	5.257	12.542	1.00	34.91
ATOM	929	CA	ASP	162	19.373	4.343	11.463	1.00	32.15
ATOM	930	CB	ASP	162	20.738	3.675	11.661	1.00	31.54
ATOM	931	CG	ASP	162	20.992	3.253	13.092	1.00	23.98
ATOM	932	OD1	ASP	162	22.164	3.334	13.510	1.00	24.51
ATOM	933	OD2	ASP	162	20.045	2.830	13.792	1.00	20.55
ATOM	934	C	ASP	162	18.259	3.311	11.457	1.00	30.83
ATOM	935	O	ASP	162	17.355	3.354	12.295	1.00	30.69
ATOM	936	N	HIS	163	18.353	2.362	10.537	1.00	28.95
ATOM	937	CA	HIS	163	17.344	1.321	10.403	1.00	24.49
ATOM	938	CB	HIS	163	17.536	0.577	9.080	1.00	21.42
ATOM	939	CG	HIS	163	17.233	1.419	7.884	1.00	14.24
ATOM	940	CD2	HIS	163	18.047	2.022	6.987	1.00	4.27
ATOM	941	ND1	HIS	163	15.944	1.765	7.532	1.00	10.79
ATOM	942	CE1	HIS	163	15.979	2.547	6.471	1.00	9.18

FIG. 1Q

ATOM	943	NE2	HIS	163	17.242	2.720	6.122	1.00	9.38
ATOM	944	C	HIS	163	17.245	0.350	11.569	1.00	18.99
ATOM	945	O	HIS	163	16.146	0.003	11.988	1.00	17.25
ATOM	946	N	GLU	164	18.381	-0.040	12.131	1.00	16.05
ATOM	947	CA	GLU	164	18.371	-0.982	13.244	1.00	21.01
ATOM	948	CB	GLU	164	19.800	-1.348	13.671	1.00	25.61
ATOM	949	CG	GLU	164	20.871	-1.297	12.549	1.00	42.31
ATOM	950	CD	GLU	164	20.424	-1.884	11.198	1.00	50.14
ATOM	951	OE1	GLU	164	19.937	-3.038	11.151	1.00	53.63
ATOM	952	OE2	GLU	164	20.576	-1.183	10.167	1.00	50.34
ATOM	953	C	GLU	164	17.575	-0.385	14.411	1.00	20.56
ATOM	954	O	GLU	164	16.705	-1.042	14.989	1.00	18.15
ATOM	955	N	ARG	165	17.816	0.893	14.689	1.00	20.23
ATOM	956	CA	ARG	165	17.123	1.597	15.755	1.00	16.22
ATOM	957	CB	ARG	165	17.782	2.948	16.028	1.00	18.25
ATOM	958	CG	ARG	165	18.675	2.981	17.264	1.00	20.28
ATOM	959	CD	ARG	165	19.244	4.370	17.508	1.00	21.80
ATOM	960	NE	ARG	165	20.669	4.460	17.180	1.00	31.00
ATOM	961	CZ	ARG	165	21.221	5.434	16.456	1.00	32.61
ATOM	962	NH1	ARG	165	20.470	6.416	15.969	1.00	33.22
ATOM	963	NH2	ARG	165	22.533	5.437	16.234	1.00	31.30
ATOM	964	C	ARG	165	15.651	1.811	15.433	1.00	16.58
ATOM	965	O	ARG	165	14.793	1.606	16.290	1.00	20.41
ATOM	966	N	MET	166	15.351	2.186	14.192	1.00	13.52
ATOM	967	CA	MET	166	13.968	2.440	13.795	1.00	10.96
ATOM	968	CB	MET	166	13.900	3.213	12.477	1.00	16.45
ATOM	969	CG	MET	166	12.457	3.530	12.024	1.00	19.78
ATOM	970	SD	MET	166	12.325	4.695	10.654	1.00	7.28
ATOM	971	CE	MET	166	14.027	5.413	10.686	1.00	2.00
ATOM	972	C	MET	166	13.107	1.193	13.701	1.00	13.90
ATOM	973	O	MET	166	11.895	1.251	13.938	1.00	10.78
ATOM	974	N	SER	167	13.714	0.075	13.307	1.00	12.74
ATOM	975	CA	SER	167	12.972	-1.178	13.210	1.00	11.00
ATOM	976	CB	SER	167	13.730	-2.231	12.381	1.00	4.79
ATOM	977	OG	SER	167	15.127	-2.242	12.637	1.00	4.90
ATOM	978	C	SER	167	12.637	-1.700	14.600	1.00	8.72
ATOM	979	O	SER	167	11.505	-2.142	14.837	1.00	9.37
ATOM	980	N	TYR	168	13.595	-1.577	15.526	1.00	10.15
ATOM	981	CA	TYR	168	13.424	-2.019	16.918	1.00	11.89
ATOM	982	CB	TYR	168	14.710	-1.851	17.723	1.00	13.12
ATOM	983	CG	TYR	168	14.653	-2.568	19.047	1.00	23.94
ATOM	984	CD1	TYR	168	14.059	-3.823	19.150	1.00	27.00
ATOM	985	CE1	TYR	168	13.986	-4.485	20.357	1.00	26.88
ATOM	986	CD2	TYR	168	15.177	-2.000	20.202	1.00	27.43
ATOM	987	CE2	TYR	168	15.105	-2.665	21.419	1.00	26.40
ATOM	988	CZ	TYR	168	14.505	-3.905	21.483	1.00	25.71
ATOM	989	OH	TYR	168	14.410	-4.560	22.678	1.00	29.78
ATOM	990	C	TYR	168	12.309	-1.281	17.638	1.00	10.11
ATOM	991	O	TYR	168	11.514	-1.894	18.352	1.00	15.94
ATOM	992	N	LEU	169	12.280	0.039	17.479	1.00	9.20
ATOM	993	CA	LEU	169	11.250	0.870	18.083	1.00	6.55
ATOM	994	CB	LEU	169	11.512	2.365	17.796	1.00	5.56
ATOM	995	CG	LEU	169	12.697	3.034	18.506	1.00	2.00
ATOM	996	CD1	LEU	169	12.942	4.395	17.946	1.00	2.00
ATOM	997	CD2	LEU	169	12.431	3.110	20.009	1.00	2.00
ATOM	998	C	LEU	169	9.896	0.464	17.526	1.00	8.60
ATOM	999	O	LEU	169	8.966	0.175	18.289	1.00	11.07
ATOM	1000	N	LEU	170	9.803	0.410	16.193	1.00	14.62
ATOM	1001	CA	LEU	170	8.563	0.035	15.516	1.00	13.43

FIG. 1R

ATOM	1002	CB	LEU	170	8.679	0.192	13.992	1.00	16.49
ATOM	1003	CG	LEU	170	8.346	1.526	13.310	1.00	8.13
ATOM	1004	CD1	LEU	170	6.970	2.026	13.733	1.00	7.52
ATOM	1005	CD2	LEU	170	9.395	2.545	13.642	1.00	12.95
ATOM	1006	C	LEU	170	8.155	-1.393	15.868	1.00	14.08
ATOM	1007	O	LEU	170	6.963	-1.695	15.974	1.00	16.12
ATOM	1008	N	TYR	171	9.139	-2.260	16.098	1.00	14.62
ATOM	1009	CA	TYR	171	8.860	-3.642	16.471	1.00	15.32
ATOM	1010	CB	TYR	171	10.156	-4.453	16.498	1.00	20.86
ATOM	1011	CG	TYR	171	10.039	-5.803	17.174	1.00	30.51
ATOM	1012	CD1	TYR	171	9.248	-6.821	16.634	1.00	29.52
ATOM	1013	CE1	TYR	171	9.120	-8.046	17.282	1.00	35.08
ATOM	1014	CD2	TYR	171	10.701	-6.054	18.375	1.00	29.23
ATOM	1015	CE2	TYR	171	10.576	-7.272	19.022	1.00	31.42
ATOM	1016	CZ	TYR	171	9.786	-8.262	18.477	1.00	34.50
ATOM	1017	OH	TYR	171	9.665	-9.464	19.133	1.00	35.71
ATOM	1018	C	TYR	171	8.174	-3.685	17.842	1.00	16.71
ATOM	1019	O	TYR	171	7.111	-4.302	17.999	1.00	22.65
ATOM	1020	N	GLN	172	8.759	-2.993	18.820	1.00	12.16
ATOM	1021	CA	GLN	172	8.207	-2.953	20.174	1.00	8.36
ATOM	1022	CB	GLN	172	9.174	-2.245	21.100	1.00	7.90
ATOM	1023	CG	GLN	172	10.537	-2.885	21.101	1.00	9.40
ATOM	1024	CD	GLN	172	11.522	-2.124	21.942	1.00	16.58
ATOM	1025	OE1	GLN	172	11.507	-2.214	23.169	1.00	25.77
ATOM	1026	NE2	GLN	172	12.382	-1.362	21.292	1.00	14.95
ATOM	1027	C	GLN	172	6.836	-2.305	20.237	1.00	6.06
ATOM	1028	O	GLN	172	5.990	-2.708	21.029	1.00	10.45
ATOM	1029	N	MET	173	6.607	-1.320	19.378	1.00	3.68
ATOM	1030	CA	MET	173	5.333	-0.635	19.332	1.00	2.37
ATOM	1031	CB	MET	173	5.400	0.520	18.335	1.00	10.38
ATOM	1032	CG	MET	173	5.939	1.827	18.917	1.00	14.77
ATOM	1033	SD	MET	173	5.978	3.168	17.706	1.00	15.09
ATOM	1034	CE	MET	173	7.699	3.414	17.615	1.00	2.00
ATOM	1035	C	MET	173	4.246	-1.615	18.940	1.00	4.64
ATOM	1036	O	MET	173	3.129	-1.572	19.462	1.00	2.00
ATOM	1037	N	LEU	174	4.603	-2.534	18.046	1.00	9.41
ATOM	1038	CA	LEU	174	3.672	-3.558	17.564	1.00	7.13
ATOM	1039	CB	LEU	174	4.151	-4.138	16.220	1.00	10.84
ATOM	1040	CG	LEU	174	4.139	-3.195	14.996	1.00	2.68
ATOM	1041	CD1	LEU	174	5.143	-3.637	13.942	1.00	5.45
ATOM	1042	CD2	LEU	174	2.752	-3.118	14.396	1.00	2.00
ATOM	1043	C	LEU	174	3.420	-4.647	18.619	1.00	3.27
ATOM	1044	O	LEU	174	2.272	-5.064	18.825	1.00	2.00
ATOM	1045	N	CYS	175	4.476	-5.096	19.299	1.00	8.94
ATOM	1046	CA	CYS	175	4.325	-6.099	20.363	1.00	5.39
ATOM	1047	CB	CYS	175	5.656	-6.386	21.040	1.00	2.00
ATOM	1048	SG	CYS	175	6.885	-7.180	20.062	1.00	9.71
ATOM	1049	C	CYS	175	3.385	-5.518	21.420	1.00	8.35
ATOM	1050	O	CYS	175	2.448	-6.184	21.872	1.00	9.82
ATOM	1051	N	GLY	176	3.630	-4.253	21.781	1.00	5.95
ATOM	1052	CA	GLY	176	2.813	-3.570	22.763	1.00	2.00
ATOM	1053	C	GLY	176	1.347	-3.517	22.374	1.00	5.44
ATOM	1054	O	GLY	176	0.489	-3.843	23.193	1.00	4.70
ATOM	1055	N	ILE	177	1.059	-3.154	21.119	1.00	8.52
ATOM	1056	CA	ILE	177	-0.321	-3.054	20.616	1.00	9.46
ATOM	1057	CB	ILE	177	-0.377	-2.276	19.274	1.00	10.93
ATOM	1058	CG2	ILE	177	-1.791	-1.785	18.997	1.00	13.45
ATOM	1059	CG1	ILE	177	0.484	-1.030	19.350	1.00	6.12
ATOM	1060	CD1	ILE	177	0.672	-0.392	18.023	1.00	12.58

FIG. 1S

ATOM	1061	C	ILE	177	-0.984	-4.425	20.422	1.00	9.48
ATOM	1062	O	ILE	177	-2.202	-4.583	20.610	1.00	2.00
ATOM	1063	N	LYS	178	-0.193	-5.424	20.054	1.00	8.60
ATOM	1064	CA	LYS	178	-0.748	-6.757	19.877	1.00	13.96
ATOM	1065	CB	LYS	178	0.275	-7.712	19.247	1.00	11.31
ATOM	1066	CG	LYS	178	-0.280	-9.093	19.037	1.00	8.75
ATOM	1067	CD	LYS	178	0.682	-9.999	18.302	1.00	13.40
ATOM	1068	CE	LYS	178	0.162	-11.436	18.309	1.00	6.81
ATOM	1069	NZ	LYS	178	-1.304	-11.536	18.017	1.00	8.76
ATOM	1070	C	LYS	178	-1.197	-7.236	21.261	1.00	12.95
ATOM	1071	O	LYS	178	-2.297	-7.773	21.406	1.00	11.31
ATOM	1072	N	HIS	179	-0.382	-6.959	22.282	1.00	14.07
ATOM	1073	CA	HIS	179	-0.720	-7.337	23.654	1.00	17.66
ATOM	1074	CB	HIS	179	0.411	-6.956	24.608	1.00	22.96
ATOM	1075	CG	HIS	179	0.252	-7.521	25.989	1.00	25.68
ATOM	1076	CD2	HIS	179	-0.527	-7.144	27.031	1.00	21.69
ATOM	1077	ND1	HIS	179	0.975	-8.606	26.430	1.00	27.24
ATOM	1078	CE1	HIS	179	0.653	-8.874	27.681	1.00	25.21
ATOM	1079	NE2	HIS	179	-0.258	-8.002	28.067	1.00	25.80
ATOM	1080	C	HIS	179	-2.010	-6.641	24.098	1.00	18.55
ATOM	1081	O	HIS	179	-2.891	-7.257	24.707	1.00	20.15
ATOM	1082	N	LEU	180	-2.130	-5.360	23.766	1.00	19.43
ATOM	1083	CA	LEU	180	-3.302	-4.570	24.125	1.00	18.86
ATOM	1084	CB	LEU	180	-3.061	-3.092	23.792	1.00	18.87
ATOM	1085	CG	LEU	180	-3.163	-2.022	24.885	1.00	17.95
ATOM	1086	CD1	LEU	180	-2.288	-2.388	26.063	1.00	16.08
ATOM	1087	CD2	LEU	180	-2.739	-0.672	24.323	1.00	19.02
ATOM	1088	C	LEU	180	-4.543	-5.075	23.400	1.00	17.60
ATOM	1089	O	LEU	180	-5.638	-5.078	23.966	1.00	16.24
ATOM	1090	N	HIS	181	-4.370	-5.498	22.148	1.00	18.47
ATOM	1091	CA	HIS	181	-5.476	-6.016	21.346	1.00	18.34
ATOM	1092	CB	HIS	181	-5.058	-6.209	19.888	1.00	22.03
ATOM	1093	CG	HIS	181	-5.010	-4.939	19.094	1.00	24.29
ATOM	1094	CD2	HIS	181	-5.866	-3.896	19.030	1.00	22.97
ATOM	1095	ND1	HIS	181	-3.972	-4.639	18.238	1.00	23.58
ATOM	1096	CE1	HIS	181	-4.194	-3.462	17.681	1.00	20.84
ATOM	1097	NE2	HIS	181	-5.335	-2.989	18.145	1.00	21.33
ATOM	1098	C	HIS	181	-5.947	-7.338	21.914	1.00	14.91
ATOM	1099	O	HIS	181	-7.142	-7.629	21.911	1.00	16.18
ATOM	1100	N	SER	182	-4.999	-8.127	22.413	1.00	16.17
ATOM	1101	CA	SER	182	-5.291	-9.425	23.011	1.00	16.47
ATOM	1102	CB	SER	182	-3.991	-10.157	23.351	1.00	12.75
ATOM	1103	OG	SER	182	-3.148	-10.271	22.215	1.00	23.12
ATOM	1104	C	SER	182	-6.094	-9.200	24.288	1.00	18.77
ATOM	1105	O	SER	182	-6.934	-10.024	24.661	1.00	24.36
ATOM	1106	N	ALA	183	-5.828	-8.070	24.945	1.00	17.65
ATOM	1107	CA	ALA	183	-6.506	-7.705	26.182	1.00	13.29
ATOM	1108	CB	ALA	183	-5.699	-6.670	26.919	1.00	13.15
ATOM	1109	C	ALA	183	-7.911	-7.183	25.911	1.00	16.33
ATOM	1110	O	ALA	183	-8.731	-7.066	26.826	1.00	22.38
ATOM	1111	N	GLY	184	-8.189	-6.883	24.646	1.00	16.47
ATOM	1112	CA	GLY	184	-9.490	-6.371	24.257	1.00	12.73
ATOM	1113	C	GLY	184	-9.461	-4.861	24.168	1.00	13.71
ATOM	1114	O	GLY	184	-10.503	-4.223	24.060	1.00	14.57
ATOM	1115	N	ILE	185	-8.256	-4.299	24.189	1.00	14.45
ATOM	1116	CA	ILE	185	-8.047	-2.856	24.141	1.00	17.69
ATOM	1117	CB	ILE	185	-7.032	-2.418	25.266	1.00	14.32
ATOM	1118	CG2	ILE	185	-6.662	-0.948	25.131	1.00	9.43
ATOM	1119	CG1	ILE	185	-7.635	-2.683	26.650	1.00	12.09

FIG. 1T

ATOM	1120	CD1	ILE	185	-6.617	-2.904	27.750	1.00	2.00
ATOM	1121	C	ILE	185	-7.555	-2.353	22.780	1.00	21.86
ATOM	1122	O	ILE	185	-6.458	-2.706	22.336	1.00	23.69
ATOM	1123	N	ILE	186	-8.401	-1.588	22.089	1.00	23.04
ATOM	1124	CA	ILE	186	-8.006	-0.998	20.810	1.00	22.05
ATOM	1125	CB	ILE	186	-9.023	-1.248	19.666	1.00	22.99
ATOM	1126	CG2	ILE	186	-8.419	-0.786	18.345	1.00	19.01
ATOM	1127	CG1	ILE	186	-9.340	-2.743	19.553	1.00	20.59
ATOM	1128	CD1	ILE	186	-10.411	-3.065	18.541	1.00	15.12
ATOM	1129	C	ILE	186	-7.832	0.503	21.068	1.00	18.01
ATOM	1130	O	ILE	186	-8.794	1.248	21.280	1.00	19.97
ATOM	1131	N	HIS	187	-6.572	0.906	21.059	1.00	11.89
ATOM	1132	CA	HIS	187	-6.143	2.266	21.331	1.00	9.65
ATOM	1133	CB	HIS	187	-4.662	2.352	21.011	1.00	7.84
ATOM	1134	CG	HIS	187	-3.903	3.274	21.898	1.00	10.36
ATOM	1135	CD2	HIS	187	-4.054	4.595	22.156	1.00	11.24
ATOM	1136	ND1	HIS	187	-2.778	2.877	22.586	1.00	13.01
ATOM	1137	CE1	HIS	187	-2.263	3.912	23.218	1.00	12.92
ATOM	1138	NE2	HIS	187	-3.015	4.964	22.975	1.00	4.76
ATOM	1139	C	HIS	187	-6.908	3.428	20.691	1.00	11.30
ATOM	1140	O	HIS	187	-7.731	4.064	21.348	1.00	13.83
ATOM	1141	N	ARG	188	-6.606	3.708	19.423	1.00	14.27
ATOM	1142	CA	ARG	188	-7.211	4.792	18.648	1.00	13.77
ATOM	1143	CB	ARG	188	-8.724	4.854	18.845	1.00	13.60
ATOM	1144	CG	ARG	188	-9.457	3.753	18.170	1.00	10.20
ATOM	1145	CD	ARG	188	-10.493	3.222	19.085	1.00	17.16
ATOM	1146	NE	ARG	188	-11.632	4.112	19.212	1.00	16.20
ATOM	1147	CZ	ARG	188	-12.508	4.040	20.206	1.00	22.11
ATOM	1148	NH1	ARG	188	-12.349	3.127	21.157	1.00	22.61
ATOM	1149	NH2	ARG	188	-13.576	4.829	20.218	1.00	21.57
ATOM	1150	C	ARG	188	-6.623	6.181	18.889	1.00	17.28
ATOM	1151	O	ARG	188	-7.229	7.173	18.501	1.00	21.13
ATOM	1152	N	ASP	189	-5.444	6.264	19.502	1.00	15.55
ATOM	1153	CA	ASP	189	-4.843	7.563	19.762	1.00	15.15
ATOM	1154	CB	ASP	189	-5.601	8.256	20.894	1.00	17.43
ATOM	1155	CG	ASP	189	-5.499	9.768	20.831	1.00	29.44
ATOM	1156	OD1	ASP	189	-5.155	10.316	19.759	1.00	36.43
ATOM	1157	OD2	ASP	189	-5.778	10.415	21.861	1.00	39.38
ATOM	1158	C	ASP	189	-3.361	7.474	20.087	1.00	15.20
ATOM	1159	O	ASP	189	-2.882	8.081	21.034	1.00	16.94
ATOM	1160	N	LEU	190	-2.632	6.747	19.255	1.00	16.38
ATOM	1161	CA	LEU	190	-1.205	6.553	19.447	1.00	14.72
ATOM	1162	CB	LEU	190	-0.753	5.278	18.741	1.00	17.54
ATOM	1163	CG	LEU	190	-0.255	4.158	19.644	1.00	12.34
ATOM	1164	CD1	LEU	190	0.027	2.938	18.825	1.00	12.26
ATOM	1165	CD2	LEU	190	1.003	4.602	20.360	1.00	13.72
ATOM	1166	C	LEU	190	-0.350	7.723	18.995	1.00	15.73
ATOM	1167	O	LEU	190	-0.118	7.906	17.805	1.00	20.11
ATOM	1168	N	LYS	191	0.098	8.527	19.954	1.00	16.43
ATOM	1169	CA	LYS	191	0.956	9.675	19.663	1.00	11.18
ATOM	1170	CB	LYS	191	0.259	10.996	20.051	1.00	15.07
ATOM	1171	CG	LYS	191	-0.201	11.126	21.516	1.00	17.28
ATOM	1172	CD	LYS	191	-1.088	12.359	21.765	1.00	10.02
ATOM	1173	CE	LYS	191	-2.531	12.116	21.321	1.00	14.89
ATOM	1174	NZ	LYS	191	-3.522	13.129	21.831	1.00	18.00
ATOM	1175	C	LYS	191	2.279	9.481	20.397	1.00	10.22
ATOM	1176	O	LYS	191	2.312	8.892	21.471	1.00	16.35
ATOM	1177	N	PRO	192	3.393	9.931	19.809	1.00	5.03
ATOM	1178	CD	PRO	192	3.460	10.575	18.493	1.00	2.00

FIG. 1U

ATOM	1179	CA	PRO	192	4.741	9.818	20.389	1.00	8.49
ATOM	1180	CB	PRO	192	5.612	10.513	19.342	1.00	9.05
ATOM	1181	CG	PRO	192	4.880	10.296	18.077	1.00	5.94
ATOM	1182	C	PRO	192	4.948	10.467	21.776	1.00	14.51
ATOM	1183	O	PRO	192	5.980	10.251	22.435	1.00	16.54
ATOM	1184	N	SER	193	3.991	11.294	22.192	1.00	13.30
ATOM	1185	CA	SER	193	4.051	11.984	23.473	1.00	14.80
ATOM	1186	CB	SER	193	3.120	13.207	23.461	1.00	14.49
ATOM	1187	OG	SER	193	1.785	12.862	23.103	1.00	8.59
ATOM	1188	C	SER	193	3.678	11.048	24.610	1.00	17.21
ATOM	1189	O	SER	193	4.047	11.279	25.763	1.00	21.39
ATOM	1190	N	ASN	194	2.938	9.999	24.258	1.00	15.65
ATOM	1191	CA	ASN	194	2.482	8.981	25.192	1.00	7.21
ATOM	1192	CB	ASN	194	1.043	8.593	24.865	1.00	7.91
ATOM	1193	CG	ASN	194	0.054	9.693	25.189	1.00	21.77
ATOM	1194	OD1	ASN	194	0.331	10.557	26.021	1.00	29.51
ATOM	1195	ND2	ASN	194	-1.118	9.658	24.561	1.00	18.85
ATOM	1196	C	ASN	194	3.371	7.742	25.091	1.00	6.70
ATOM	1197	O	ASN	194	2.964	6.651	25.476	1.00	8.40
ATOM	1198	N	ILE	195	4.580	7.908	24.564	1.00	2.00
ATOM	1199	CA	ILE	195	5.507	6.798	24.397	1.00	2.73
ATOM	1200	CB	ILE	195	5.625	6.355	22.899	1.00	5.68
ATOM	1201	CG2	ILE	195	6.725	5.321	22.732	1.00	2.00
ATOM	1202	CG1	ILE	195	4.295	5.789	22.397	1.00	2.00
ATOM	1203	CD1	ILE	195	4.313	5.374	20.938	1.00	6.01
ATOM	1204	C	ILE	195	6.858	7.244	24.903	1.00	3.99
ATOM	1205	O	ILE	195	7.315	8.341	24.584	1.00	8.39
ATOM	1206	N	VAL	196	7.500	6.375	25.676	1.00	5.82
ATOM	1207	CA	VAL	196	8.803	6.663	26.270	1.00	11.18
ATOM	1208	CB	VAL	196	8.682	6.901	27.805	1.00	13.47
ATOM	1209	CG1	VAL	196	8.198	8.316	28.079	1.00	10.74
ATOM	1210	CG2	VAL	196	7.692	5.913	28.430	1.00	14.45
ATOM	1211	C	VAL	196	9.829	5.574	25.971	1.00	10.32
ATOM	1212	O	VAL	196	9.479	4.403	25.825	1.00	21.42
ATOM	1213	N	VAL	197	11.089	5.971	25.808	1.00	5.51
ATOM	1214	CA	VAL	197	12.158	5.027	25.502	1.00	4.80
ATOM	1215	CB	VAL	197	12.639	5.133	24.002	1.00	10.58
ATOM	1216	CG1	VAL	197	11.531	5.695	23.102	1.00	6.44
ATOM	1217	CG2	VAL	197	13.920	5.945	23.856	1.00	4.90
ATOM	1218	C	VAL	197	13.334	5.191	26.454	1.00	7.69
ATOM	1219	O	VAL	197	13.406	6.158	27.209	1.00	10.91
ATOM	1220	N	LYS	198	14.270	4.250	26.390	1.00	10.12
ATOM	1221	CA	LYS	198	15.442	4.243	27.254	1.00	11.52
ATOM	1222	CB	LYS	198	15.386	3.003	28.149	1.00	16.60
ATOM	1223	CG	LYS	198	16.189	3.136	29.427	1.00	26.28
ATOM	1224	CD	LYS	198	16.150	1.878	30.272	1.00	31.00
ATOM	1225	CE	LYS	198	14.768	1.615	30.854	1.00	37.45
ATOM	1226	NZ	LYS	198	14.780	0.433	31.779	1.00	39.49
ATOM	1227	C	LYS	198	16.712	4.240	26.403	1.00	16.21
ATOM	1228	O	LYS	198	16.637	4.095	25.187	1.00	17.79
ATOM	1229	N	SER	199	17.876	4.367	27.040	1.00	17.91
ATOM	1230	CA	SER	199	19.152	4.397	26.328	1.00	18.09
ATOM	1231	CB	SER	199	20.308	4.677	27.280	1.00	17.32
ATOM	1232	OG	SER	199	20.405	6.068	27.526	1.00	22.33
ATOM	1233	C	SER	199	19.475	3.190	25.447	1.00	20.05
ATOM	1234	O	SER	199	20.301	3.285	24.548	1.00	21.63
ATOM	1235	N	ASP	200	18.864	2.045	25.727	1.00	21.10
ATOM	1236	CA	ASP	200	19.086	0.872	24.891	1.00	17.62
ATOM	1237	CB	ASP	200	19.288	-0.408	25.724	1.00	14.14

FIG. 1V

ATOM	1238	CG	ASP	200	18.209	-0.625	26.779	1.00	13.05
ATOM	1239	OD1	ASP	200	17.051	-0.223	26.574	1.00	10.97
ATOM	1240	OD2	ASP	200	18.528	-1.231	27.822	1.00	13.20
ATOM	1241	C	ASP	200	17.875	0.776	23.977	1.00	18.24
ATOM	1242	O	ASP	200	17.465	-0.298	23.559	1.00	22.86
ATOM	1243	N	CYS	201	17.283	1.936	23.723	1.00	18.66
ATOM	1244	CA	CYS	201	16.114	2.071	22.870	1.00	21.37
ATOM	1245	CB	CYS	201	16.491	1.963	21.378	1.00	22.84
ATOM	1246	SG	CYS	201	17.104	3.519	20.591	1.00	22.39
ATOM	1247	C	CYS	201	14.929	1.170	23.205	1.00	20.00
ATOM	1248	O	CYS	201	14.077	0.934	22.347	1.00	25.61
ATOM	1249	N	THR	202	14.862	0.658	24.437	1.00	15.48
ATOM	1250	CA	THR	202	13.715	-0.174	24.815	1.00	15.71
ATOM	1251	CB	THR	202	13.954	-0.996	26.087	1.00	15.14
ATOM	1252	OG1	THR	202	14.531	-0.171	27.107	1.00	24.66
ATOM	1253	CG2	THR	202	14.881	-2.163	25.780	1.00	16.97
ATOM	1254	C	THR	202	12.539	0.772	24.963	1.00	12.64
ATOM	1255	O	THR	202	12.694	1.884	25.454	1.00	18.75
ATOM	1256	N	LEU	203	11.370	0.343	24.513	1.00	11.71
ATOM	1257	CA	LEU	203	10.192	1.202	24.507	1.00	11.07
ATOM	1258	CB	LEU	203	9.790	1.396	23.035	1.00	7.87
ATOM	1259	CG	LEU	203	8.550	2.108	22.503	1.00	8.82
ATOM	1260	CD1	LEU	203	8.821	2.537	21.066	1.00	6.21
ATOM	1261	CD2	LEU	203	7.330	1.200	22.578	1.00	2.00
ATOM	1262	C	LEU	203	8.994	0.752	25.339	1.00	12.47
ATOM	1263	O	LEU	203	8.834	-0.436	25.628	1.00	17.72
ATOM	1264	N	LYS	204	8.134	1.720	25.668	1.00	3.95
ATOM	1265	CA	LYS	204	6.923	1.496	26.443	1.00	2.00
ATOM	1266	CB	LYS	204	7.184	1.693	27.944	1.00	3.61
ATOM	1267	CG	LYS	204	7.814	0.487	28.650	1.00	6.82
ATOM	1268	CD	LYS	204	8.128	0.807	30.098	1.00	8.75
ATOM	1269	CE	LYS	204	9.139	-0.175	30.683	1.00	10.28
ATOM	1270	NZ	LYS	204	8.520	-1.437	31.124	1.00	8.47
ATOM	1271	C	LYS	204	5.854	2.477	25.996	1.00	2.00
ATOM	1272	O	LYS	204	6.154	3.620	25.687	1.00	3.81
ATOM	1273	N	ILE	205	4.617	2.007	25.921	1.00	2.00
ATOM	1274	CA	ILE	205	3.479	2.830	25.538	1.00	3.79
ATOM	1275	CB	ILE	205	2.498	2.070	24.610	1.00	6.77
ATOM	1276	CG2	ILE	205	1.214	2.877	24.403	1.00	2.00
ATOM	1277	CG1	ILE	205	3.167	1.763	23.270	1.00	7.79
ATOM	1278	CD1	ILE	205	2.238	1.080	22.284	1.00	7.74
ATOM	1279	C	ILE	205	2.751	3.138	26.834	1.00	11.47
ATOM	1280	O	ILE	205	2.189	2.244	27.462	1.00	13.38
ATOM	1281	N	LEU	206	2.667	4.418	27.165	1.00	12.52
ATOM	1282	CA	LEU	206	2.048	4.852	28.401	1.00	13.05
ATOM	1283	CB	LEU	206	2.527	6.264	28.749	1.00	15.77
ATOM	1284	CG	LEU	206	4.040	6.517	28.734	1.00	16.73
ATOM	1285	CD1	LEU	206	4.274	8.008	28.716	1.00	17.19
ATOM	1286	CD2	LEU	206	4.747	5.874	29.918	1.00	14.95
ATOM	1287	C	LEU	206	0.536	4.766	28.542	1.00	14.20
ATOM	1288	O	LEU	206	0.064	4.541	29.655	1.00	19.67
ATOM	1289	N	ASP	207	-0.236	4.883	27.462	1.00	10.78
ATOM	1290	CA	ASP	207	-1.692	4.853	27.636	1.00	10.76
ATOM	1291	CB	ASP	207	-2.280	6.235	27.335	1.00	14.80
ATOM	1292	CG	ASP	207	-2.281	6.575	25.851	1.00	22.89
ATOM	1293	OD1	ASP	207	-3.373	6.921	25.335	1.00	22.44
ATOM	1294	OD2	ASP	207	-1.204	6.511	25.210	1.00	21.36
ATOM	1295	C	ASP	207	-2.507	3.764	26.937	1.00	11.69
ATOM	1296	O	ASP	207	-1.956	2.926	26.223	1.00	15.31

FIG. 1W

ATOM	1297	N	PHE	208	-3.819	3.776	27.179	1.00	7.76
ATOM	1298	CA	PHE	208	-4.739	2.809	26.593	1.00	7.38
ATOM	1299	CB	PHE	208	-5.458	2.005	27.688	1.00	12.69
ATOM	1300	CG	PHE	208	-4.514	1.331	28.648	1.00	11.63
ATOM	1301	CD1	PHE	208	-4.326	1.833	29.932	1.00	19.85
ATOM	1302	CD2	PHE	208	-3.753	0.251	28.240	1.00	12.07
ATOM	1303	CE1	PHE	208	-3.368	1.269	30.793	1.00	16.31
ATOM	1304	CE2	PHE	208	-2.797	-0.323	29.080	1.00	14.94
ATOM	1305	CZ	PHE	208	-2.600	0.190	30.363	1.00	14.41
ATOM	1306	C	PHE	208	-5.738	3.488	25.669	1.00	10.81
ATOM	1307	O	PHE	208	-6.769	2.917	25.326	1.00	7.83
ATOM	1308	N	GLY	209	-5.457	4.749	25.345	1.00	14.37
ATOM	1309	CA	GLY	209	-6.269	5.515	24.414	1.00	11.22
ATOM	1310	C	GLY	209	-7.711	5.857	24.716	1.00	14.15
ATOM	1311	O	GLY	209	-8.073	6.130	25.864	1.00	16.16
ATOM	1312	N	LEU	210	-8.530	5.835	23.661	1.00	15.03
ATOM	1313	CA	LEU	210	-9.958	6.173	23.725	1.00	19.13
ATOM	1314	CB	LEU	210	-10.429	6.677	22.362	1.00	18.59
ATOM	1315	CG	LEU	210	-9.546	7.639	21.575	1.00	21.21
ATOM	1316	CD1	LEU	210	-10.096	7.786	20.162	1.00	21.04
ATOM	1317	CD2	LEU	210	-9.479	8.981	22.283	1.00	21.95
ATOM	1318	C	LEU	210	-10.895	5.048	24.140	1.00	23.06
ATOM	1319	O	LEU	210	-10.631	3.871	23.886	1.00	27.54
ATOM	1320	N	ALA	211	-12.023	5.428	24.730	1.00	26.46
ATOM	1321	CA	ALA	211	-13.029	4.460	25.152	1.00	31.93
ATOM	1322	CB	ALA	211	-13.833	5.013	26.324	1.00	33.70
ATOM	1323	C	ALA	211	-13.938	4.200	23.954	1.00	37.57
ATOM	1324	O	ALA	211	-14.160	5.102	23.140	1.00	39.41
ATOM	1325	N	ALA	212	-14.456	2.975	23.848	1.00	41.47
ATOM	1326	CA	ALA	212	-15.334	2.574	22.741	1.00	44.00
ATOM	1327	CB	ALA	212	-15.865	1.170	22.987	1.00	40.73
ATOM	1328	C	ALA	212	-16.494	3.539	22.457	1.00	46.85
ATOM	1329	O	ALA	212	-16.590	4.009	21.294	1.00	45.16
ATOM	1330	CB	VAL	225	-9.000	18.138	19.811	1.00	38.33
ATOM	1331	CG1	VAL	225	-8.808	16.791	20.485	1.00	36.84
ATOM	1332	CG2	VAL	225	-10.183	18.882	20.426	1.00	33.61
ATOM	1333	C	VAL	225	-6.661	18.403	18.962	1.00	46.33
ATOM	1334	O	VAL	225	-6.466	18.939	17.870	1.00	51.16
ATOM	1335	N	VAL	225	-7.928	20.395	19.562	1.00	45.47
ATOM	1336	CA	VAL	225	-7.699	18.972	19.928	1.00	42.53
ATOM	1337	N	THR	226	-5.978	17.340	19.378	1.00	47.37
ATOM	1338	CA	THR	226	-4.959	16.692	18.550	1.00	43.20
ATOM	1339	CB	THR	226	-3.798	16.159	19.417	1.00	45.47
ATOM	1340	OG1	THR	226	-3.273	17.220	20.231	1.00	44.76
ATOM	1341	CG2	THR	226	-2.690	15.583	18.538	1.00	41.66
ATOM	1342	C	THR	226	-5.544	15.517	17.770	1.00	41.24
ATOM	1343	O	THR	226	-6.141	14.608	18.355	1.00	41.37
ATOM	1344	N	ALA	227	-5.360	15.533	16.455	1.00	37.27
ATOM	1345	CA	ALA	227	-5.862	14.461	15.610	1.00	31.23
ATOM	1346	CB	ALA	227	-7.220	14.841	15.019	1.00	23.57
ATOM	1347	C	ALA	227	-4.868	14.132	14.500	1.00	27.64
ATOM	1348	O	ALA	227	-5.232	13.478	13.526	1.00	30.70
ATOM	1349	N	TYR	228	-3.612	14.552	14.667	1.00	24.30
ATOM	1350	CA	TYR	228	-2.575	14.312	13.652	1.00	23.17
ATOM	1351	CB	TYR	228	-1.246	14.990	14.007	1.00	21.58
ATOM	1352	CG	TYR	228	-1.291	16.467	14.284	1.00	23.46
ATOM	1353	CD1	TYR	228	-0.197	17.108	14.858	1.00	21.86
ATOM	1354	CE1	TYR	228	-0.219	18.457	15.136	1.00	27.59
ATOM	1355	CD2	TYR	228	-2.416	17.229	13.991	1.00	22.69

FIG. 1X

ATOM	1356	CE2	TYR	228	-2.448	18.587	14.265	1.00	30.74
ATOM	1357	CZ	TYR	228	-1.344	19.196	14.838	1.00	32.92
ATOM	1358	OH	TYR	228	-1.366	20.546	15.102	1.00	39.97
ATOM	1359	C	TYR	228	-2.260	12.829	13.438	1.00	24.23
ATOM	1360	O	TYR	228	-1.750	12.451	12.379	1.00	25.15
ATOM	1361	N	TYR	229	-2.525	12.000	14.449	1.00	23.04
ATOM	1362	CA	TYR	229	-2.204	10.575	14.355	1.00	17.62
ATOM	1363	CB	TYR	229	-1.270	10.177	15.503	1.00	15.95
ATOM	1364	CG	TYR	229	0.000	10.991	15.552	1.00	7.25
ATOM	1365	CD1	TYR	229	-0.005	12.295	16.034	1.00	7.16
ATOM	1366	CE1	TYR	229	1.151	13.057	16.045	1.00	2.00
ATOM	1367	CD2	TYR	229	1.204	10.472	15.092	1.00	2.00
ATOM	1368	CE2	TYR	229	2.367	11.234	15.101	1.00	2.00
ATOM	1369	CZ	TYR	229	2.326	12.520	15.580	1.00	3.35
ATOM	1370	OH	TYR	229	3.451	13.286	15.593	1.00	7.73
ATOM	1371	C	TYR	229	-3.410	9.647	14.305	1.00	17.31
ATOM	1372	O	TYR	229	-3.267	8.427	14.212	1.00	14.75
ATOM	1373	N	ARG	230	-4.602	10.226	14.314	1.00	19.16
ATOM	1374	CA	ARG	230	-5.818	9.426	14.268	1.00	23.52
ATOM	1375	CB	ARG	230	-6.995	10.208	14.865	1.00	23.61
ATOM	1376	CG	ARG	230	-6.688	10.667	16.293	1.00	28.96
ATOM	1377	CD	ARG	230	-7.900	11.083	17.092	1.00	30.92
ATOM	1378	NE	ARG	230	-7.468	11.590	18.395	1.00	34.96
ATOM	1379	CZ	ARG	230	-8.274	11.863	19.418	1.00	36.46
ATOM	1380	NH1	ARG	230	-9.585	11.685	19.319	1.00	37.33
ATOM	1381	NH2	ARG	230	-7.760	12.341	20.544	1.00	35.13
ATOM	1382	C	ARG	230	-6.117	8.922	12.849	1.00	26.24
ATOM	1383	O	ARG	230	-5.851	9.605	11.850	1.00	29.78
ATOM	1384	N	ALA	231	-6.648	7.706	12.788	1.00	22.73
ATOM	1385	CA	ALA	231	-6.968	7.037	11.531	1.00	18.49
ATOM	1386	CB	ALA	231	-7.110	5.543	11.755	1.00	15.82
ATOM	1387	C	ALA	231	-8.230	7.596	10.886	1.00	16.95
ATOM	1388	O	ALA	231	-9.102	8.128	11.567	1.00	19.43
ATOM	1389	N	PRO	232	-8.352	7.458	9.556	1.00	13.15
ATOM	1390	CD	PRO	232	-7.287	6.952	8.668	1.00	10.64
ATOM	1391	CA	PRO	232	-9.488	7.930	8.767	1.00	8.39
ATOM	1392	CB	PRO	232	-9.153	7.395	7.373	1.00	9.88
ATOM	1393	CG	PRO	232	-7.654	7.536	7.325	1.00	6.53
ATOM	1394	C	PRO	232	-10.852	7.463	9.254	1.00	9.91
ATOM	1395	O	PRO	232	-11.823	8.220	9.229	1.00	4.70
ATOM	1396	N	GLU	233	-10.908	6.223	9.744	1.00	16.52
ATOM	1397	CA	GLU	233	-12.157	5.636	10.238	1.00	17.87
ATOM	1398	CB	GLU	233	-12.083	4.097	10.278	1.00	17.61
ATOM	1399	CG	GLU	233	-11.054	3.502	11.228	1.00	24.07
ATOM	1400	CD	GLU	233	-9.764	3.091	10.545	1.00	23.95
ATOM	1401	OE1	GLU	233	-9.227	3.891	9.762	1.00	32.58
ATOM	1402	OE2	GLU	233	-9.283	1.964	10.787	1.00	20.43
ATOM	1403	C	GLU	233	-12.584	6.193	11.593	1.00	21.23
ATOM	1404	O	GLU	233	-13.756	6.081	11.974	1.00	22.33
ATOM	1405	N	VAL	234	-11.636	6.786	12.319	1.00	19.53
ATOM	1406	CA	VAL	234	-11.920	7.393	13.611	1.00	16.80
ATOM	1407	CB	VAL	234	-10.672	7.385	14.529	1.00	15.57
ATOM	1408	CG1	VAL	234	-10.978	8.082	15.841	1.00	20.84
ATOM	1409	CG2	VAL	234	-10.235	5.956	14.793	1.00	17.05
ATOM	1410	C	VAL	234	-12.356	8.837	13.334	1.00	19.12
ATOM	1411	O	VAL	234	-13.415	9.268	13.798	1.00	21.96
ATOM	1412	N	ILE	235	-11.580	9.552	12.515	1.00	19.93
ATOM	1413	CA	ILE	235	-11.889	10.935	12.129	1.00	14.90
ATOM	1414	CB	ILE	235	-10.856	11.507	11.116	1.00	6.48

FIG. 1Y

ATOM	1415	CG2	ILE	235	-11.216	12.918	10.742	1.00	11.04
ATOM	1416	CG1	ILE	235	-9.439	11.479	11.682	1.00	3.71
ATOM	1417	CD1	ILE	235	-8.390	11.912	10.670	1.00	2.00
ATOM	1418	C	ILE	235	-13.255	11.029	11.447	1.00	16.32
ATOM	1419	O	ILE	235	-13.968	12.015	11.618	1.00	21.85
ATOM	1420	N	LEU	236	-13.600	10.021	10.647	1.00	20.37
ATOM	1421	CA	LEU	236	-14.871	10.025	9.921	1.00	21.61
ATOM	1422	CB	LEU	236	-14.652	9.597	8.469	1.00	17.45
ATOM	1423	CG	LEU	236	-13.731	10.515	7.653	1.00	21.12
ATOM	1424	CD1	LEU	236	-13.497	9.937	6.275	1.00	19.91
ATOM	1425	CD2	LEU	236	-14.315	11.913	7.533	1.00	17.10
ATOM	1426	C	LEU	236	-15.990	9.212	10.566	1.00	23.24
ATOM	1427	O	LEU	236	-17.148	9.325	10.175	1.00	23.76
ATOM	1428	N	GLY	237	-15.638	8.410	11.567	1.00	29.40
ATOM	1429	CA	GLY	237	-16.611	7.597	12.277	1.00	29.75
ATOM	1430	C	GLY	237	-17.297	6.528	11.457	1.00	31.11
ATOM	1431	O	GLY	237	-18.505	6.598	11.220	1.00	31.67
ATOM	1432	N	MET	238	-16.530	5.528	11.034	1.00	33.24
ATOM	1433	CA	MET	238	-17.072	4.430	10.232	1.00	40.35
ATOM	1434	CB	MET	238	-16.294	4.322	8.911	1.00	42.67
ATOM	1435	CG	MET	238	-16.364	5.541	8.015	1.00	43.24
ATOM	1436	SD	MET	238	-15.094	5.451	6.744	1.00	45.00
ATOM	1437	CE	MET	238	-13.860	6.403	7.497	1.00	45.15
ATOM	1438	C	MET	238	-16.997	3.081	10.958	1.00	38.94
ATOM	1439	O	MET	238	-17.393	2.045	10.410	1.00	41.45
ATOM	1440	N	GLY	239	-16.535	3.098	12.203	1.00	35.34
ATOM	1441	CA	GLY	239	-16.375	1.855	12.935	1.00	32.28
ATOM	1442	C	GLY	239	-14.904	1.531	12.758	1.00	28.98
ATOM	1443	O	GLY	239	-14.227	2.181	11.949	1.00	31.47
ATOM	1444	N	TYR	240	-14.400	0.518	13.454	1.00	23.63
ATOM	1445	CA	TYR	240	-12.976	0.208	13.356	1.00	14.17
ATOM	1446	CB	TYR	240	-12.192	1.131	14.309	1.00	20.41
ATOM	1447	CG	TYR	240	-12.658	1.072	15.757	1.00	23.03
ATOM	1448	CD1	TYR	240	-11.957	0.341	16.711	1.00	18.92
ATOM	1449	CE1	TYR	240	-12.412	0.252	18.031	1.00	18.94
ATOM	1450	CD2	TYR	240	-13.826	1.720	16.165	1.00	22.91
ATOM	1451	CE2	TYR	240	-14.282	1.633	17.484	1.00	23.42
ATOM	1452	CZ	TYR	240	-13.573	0.896	18.405	1.00	23.41
ATOM	1453	OH	TYR	240	-14.041	0.786	19.693	1.00	31.32
ATOM	1454	C	TYR	240	-12.668	-1.236	13.699	1.00	12.19
ATOM	1455	O	TYR	240	-13.571	-2.027	14.019	1.00	10.14
ATOM	1456	N	LYS	241	-11.384	-1.572	13.613	1.00	3.54
ATOM	1457	CA	LYS	241	-10.892	-2.896	13.956	1.00	6.13
ATOM	1458	CB	LYS	241	-11.100	-3.908	12.811	1.00	8.75
ATOM	1459	CG	LYS	241	-10.067	-3.898	11.690	1.00	10.54
ATOM	1460	CD	LYS	241	-10.537	-4.791	10.543	1.00	11.62
ATOM	1461	CE	LYS	241	-9.530	-4.846	9.401	1.00	11.38
ATOM	1462	NZ	LYS	241	-10.032	-5.638	8.231	1.00	21.31
ATOM	1463	C	LYS	241	-9.430	-2.764	14.368	1.00	5.59
ATOM	1464	O	LYS	241	-8.872	-1.673	14.342	1.00	6.19
ATOM	1465	N	GLU	242	-8.804	-3.869	14.739	1.00	9.26
ATOM	1466	CA	GLU	242	-7.423	-3.833	15.198	1.00	12.44
ATOM	1467	CB	GLU	242	-6.847	-5.242	15.424	1.00	11.72
ATOM	1468	CG	GLU	242	-7.788	-6.420	15.179	1.00	17.26
ATOM	1469	CD	GLU	242	-8.706	-6.728	16.343	1.00	13.46
ATOM	1470	OE1	GLU	242	-8.191	-6.923	17.456	1.00	20.43
ATOM	1471	OE2	GLU	242	-9.937	-6.812	16.140	1.00	15.86
ATOM	1472	C	GLU	242	-6.444	-3.021	14.369	1.00	14.72
ATOM	1473	O	GLU	242	-5.565	-2.372	14.926	1.00	21.41

FIG. 1Z

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ATOM   1474  N   ASN  243      -6.587  -3.013  13.050  1.00  19.31
ATOM   1475  CA  ASN  243      -5.613  -2.277  12.248  1.00  21.03
ATOM   1476  CB  ASN  243      -5.559  -2.800  10.799  1.00  21.90
ATOM   1477  CG  ASN  243      -6.795  -2.463   9.992  1.00  22.02
ATOM   1478  OD1 ASN  243      -7.752  -1.884  10.502  1.00  25.24
ATOM   1479  ND2 ASN  243      -6.770  -2.811   8.713  1.00  26.83
ATOM   1480  C   ASN  243      -5.729  -0.752  12.318  1.00  19.59
ATOM   1481  O   ASN  243      -4.985  -0.033  11.651  1.00  21.35
ATOM   1482  N   VAL  244      -6.609  -0.254  13.180  1.00  16.86
ATOM   1483  CA  VAL  244      -6.764   1.183  13.322  1.00  12.16
ATOM   1484  CB  VAL  244      -8.023   1.555  14.132  1.00   6.16
ATOM   1485  CG1 VAL  244      -7.913   1.067  15.554  1.00   5.57
ATOM   1486  CG2 VAL  244      -8.271   3.048  14.067  1.00   3.91
ATOM   1487  C   VAL  244      -5.517   1.766  13.967  1.00  12.08
ATOM   1488  O   VAL  244      -5.170   2.921  13.738  1.00  17.02
ATOM   1489  N   ASP  245      -4.800   0.934  14.714  1.00  10.69
ATOM   1490  CA  ASP  245      -3.578   1.372  15.378  1.00   7.76
ATOM   1491  CB  ASP  245      -3.309   0.543  16.641  1.00  14.73
ATOM   1492  CG  ASP  245      -4.325   0.794  17.735  1.00  15.38
ATOM   1493  OD1 ASP  245      -4.728   1.967  17.889  1.00  14.39
ATOM   1494  OD2 ASP  245      -4.720  -0.170  18.426  1.00   9.85
ATOM   1495  C   ASP  245      -2.399   1.252  14.460  1.00   5.82
ATOM   1496  O   ASP  245      -1.287   1.611  14.832  1.00   8.10
ATOM   1497  N   ILE  246      -2.611   0.662  13.291  1.00  11.60
ATOM   1498  CA  ILE  246      -1.529   0.509  12.318  1.00  14.99
ATOM   1499  CB  ILE  246      -1.806  -0.674  11.316  1.00  15.80
ATOM   1500  CG2 ILE  246      -0.951  -0.557  10.049  1.00  17.53
ATOM   1501  CG1 ILE  246      -1.498  -2.014  11.999  1.00   9.33
ATOM   1502  CD1 ILE  246      -0.022  -2.248  12.261  1.00   2.50
ATOM   1503  C   ILE  246      -1.310   1.847  11.599  1.00  11.65
ATOM   1504  O   ILE  246      -0.174   2.223  11.300  1.00  12.98
ATOM   1505  N   TRP  247      -2.390   2.607  11.422  1.00  13.04
ATOM   1506  CA  TRP  247      -2.305   3.913  10.784  1.00  13.02
ATOM   1507  CB  TRP  247      -3.670   4.593  10.747  1.00  15.24
ATOM   1508  CG  TRP  247      -3.591   6.016  10.254  1.00  25.04
ATOM   1509  CD2 TRP  247      -3.678   6.466   8.891  1.00  29.15
ATOM   1510  CE2 TRP  247      -3.507   7.868   8.903  1.00  32.78
ATOM   1511  CE3 TRP  247      -3.872   5.820   7.666  1.00  27.68
ATOM   1512  CD1 TRP  247      -3.382   7.144  11.010  1.00  24.32
ATOM   1513  NE1 TRP  247      -3.332   8.254  10.209  1.00  22.09
ATOM   1514  CZ2 TRP  247      -3.527   8.635   7.723  1.00  33.21
ATOM   1515  CZ3 TRP  247      -3.894   6.578   6.504  1.00  23.18
ATOM   1516  CH2 TRP  247      -3.721   7.967   6.538  1.00  27.77
ATOM   1517  C   TRP  247      -1.345   4.789  11.577  1.00  15.01
ATOM   1518  O   TRP  247      -0.313   5.238  11.065  1.00  16.99
ATOM   1519  N   SER  248      -1.662   4.948  12.860  1.00  14.45
ATOM   1520  CA  SER  248      -0.891   5.771  13.784  1.00  12.48
ATOM   1521  CB  SER  248      -1.533   5.716  15.168  1.00  13.86
ATOM   1522  OG  SER  248      -2.952   5.797  15.062  1.00  13.99
ATOM   1523  C   SER  248       0.580   5.370  13.850  1.00  11.77
ATOM   1524  O   SER  248       1.449   6.225  14.042  1.00  16.52
ATOM   1525  N   VAL  249       0.865   4.080  13.681  1.00  11.99
ATOM   1526  CA  VAL  249       2.247   3.581  13.698  1.00   8.92
ATOM   1527  CB  VAL  249       2.304   2.027  13.853  1.00  11.36
ATOM   1528  CG1 VAL  249       3.735   1.528  13.770  1.00   6.01
ATOM   1529  CG2 VAL  249       1.674   1.599  15.181  1.00  10.49
ATOM   1530  C   VAL  249       2.901   3.985  12.378  1.00  11.02
ATOM   1531  O   VAL  249       4.125   4.165  12.291  1.00   7.81
ATOM   1532  N   GLY  250       2.065   4.121  11.351  1.00   6.91
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FIG. 1AA

ATOM	1533	CA	GLY	250	2.548	4.527	10.047	1.00	5.35
ATOM	1534	C	GLY	250	2.963	5.977	10.119	1.00	4.31
ATOM	1535	O	GLY	250	4.077	6.338	9.724	1.00	4.22
ATOM	1536	N	CYS	251	2.076	6.799	10.678	1.00	7.44
ATOM	1537	CA	CYS	251	2.312	8.230	10.856	1.00	2.00
ATOM	1538	CB	CYS	251	1.138	8.858	11.601	1.00	2.00
ATOM	1539	SG	CYS	251	-0.474	8.661	10.799	1.00	2.78
ATOM	1540	C	CYS	251	3.616	8.467	11.631	1.00	6.97
ATOM	1541	O	CYS	251	4.438	9.292	11.231	1.00	12.60
ATOM	1542	N	ILE	252	3.823	7.706	12.709	1.00	7.61
ATOM	1543	CA	ILE	252	5.019	7.810	13.556	1.00	6.09
ATOM	1544	CB	ILE	252	4.871	6.950	14.831	1.00	4.83
ATOM	1545	CG2	ILE	252	6.218	6.808	15.530	1.00	2.00
ATOM	1546	CG1	ILE	252	3.785	7.533	15.739	1.00	9.15
ATOM	1547	CD1	ILE	252	3.368	6.618	16.876	1.00	8.65
ATOM	1548	C	ILE	252	6.274	7.349	12.827	1.00	6.13
ATOM	1549	O	ILE	252	7.345	7.934	12.981	1.00	8.25
ATOM	1550	N	MET	253	6.147	6.255	12.083	1.00	12.21
ATOM	1551	CA	MET	253	7.260	5.700	11.321	1.00	9.31
ATOM	1552	CB	MET	253	6.843	4.378	10.689	1.00	12.07
ATOM	1553	CG	MET	253	7.951	3.710	9.911	1.00	17.77
ATOM	1554	SD	MET	253	7.378	2.346	8.895	1.00	14.25
ATOM	1555	CE	MET	253	8.981	1.704	8.404	1.00	2.00
ATOM	1556	C	MET	253	7.670	6.688	10.230	1.00	6.53
ATOM	1557	O	MET	253	8.856	6.991	10.063	1.00	6.83
ATOM	1558	N	GLY	254	6.674	7.231	9.530	1.00	7.59
ATOM	1559	CA	GLY	254	6.927	8.196	8.473	1.00	14.92
ATOM	1560	C	GLY	254	7.597	9.453	9.010	1.00	19.52
ATOM	1561	O	GLY	254	8.446	10.057	8.346	1.00	22.42
ATOM	1562	N	GLU	255	7.242	9.813	10.240	1.00	15.34
ATOM	1563	CA	GLU	255	7.779	10.975	10.924	1.00	8.43
ATOM	1564	CB	GLU	255	6.897	11.265	12.124	1.00	10.24
ATOM	1565	CG	GLU	255	7.168	12.568	12.834	1.00	6.53
ATOM	1566	CD	GLU	255	6.188	12.798	13.961	1.00	8.13
ATOM	1567	OE1	GLU	255	4.984	12.542	13.770	1.00	11.86
ATOM	1568	OE2	GLU	255	6.616	13.241	15.034	1.00	16.77
ATOM	1569	C	GLU	255	9.219	10.734	11.369	1.00	6.94
ATOM	1570	O	GLU	255	10.010	11.670	11.503	1.00	7.55
ATOM	1571	N	MET	256	9.575	9.475	11.584	1.00	10.29
ATOM	1572	CA	MET	256	10.926	9.155	12.008	1.00	14.75
ATOM	1573	CB	MET	256	11.005	7.723	12.561	1.00	15.70
ATOM	1574	CG	MET	256	10.308	7.560	13.918	1.00	17.40
ATOM	1575	SD	MET	256	10.091	5.868	14.551	1.00	20.23
ATOM	1576	CE	MET	256	11.669	5.577	15.143	1.00	5.04
ATOM	1577	C	MET	256	11.889	9.368	10.854	1.00	13.20
ATOM	1578	O	MET	256	13.065	9.670	11.069	1.00	15.06
ATOM	1579	N	VAL	257	11.383	9.226	9.630	1.00	18.22
ATOM	1580	CA	VAL	257	12.204	9.418	8.436	1.00	17.33
ATOM	1581	CB	VAL	257	11.888	8.413	7.292	1.00	10.85
ATOM	1582	CG1	VAL	257	12.854	7.265	7.338	1.00	16.21
ATOM	1583	CG2	VAL	257	10.486	7.908	7.389	1.00	7.85
ATOM	1584	C	VAL	257	12.095	10.834	7.884	1.00	18.77
ATOM	1585	O	VAL	257	13.087	11.405	7.432	1.00	22.01
ATOM	1586	N	ARG	258	10.902	11.414	7.950	1.00	17.51
ATOM	1587	CA	ARG	258	10.687	12.761	7.447	1.00	22.55
ATOM	1588	CB	ARG	258	9.202	12.972	7.127	1.00	22.92
ATOM	1589	CG	ARG	258	8.928	14.159	6.230	1.00	22.96
ATOM	1590	CD	ARG	258	7.457	14.274	5.883	1.00	28.64
ATOM	1591	NE	ARG	258	7.054	13.466	4.727	1.00	28.26

FIG. 1BB

ATOM	1592	CZ	ARG	258	5.796	13.362	4.296	1.00	26.76
ATOM	1593	NH1	ARG	258	4.824	14.004	4.930	1.00	28.87
ATOM	1594	NH2	ARG	258	5.509	12.661	3.207	1.00	24.96
ATOM	1595	C	ARG	258	11.173	13.806	8.456	1.00	25.86
ATOM	1596	O	ARG	258	11.658	14.870	8.070	1.00	32.18
ATOM	1597	N	HIS	259	11.109	13.446	9.740	1.00	24.12
ATOM	1598	CA	HIS	259	11.494	14.313	10.857	1.00	22.37
ATOM	1599	CB	HIS	259	12.851	14.986	10.603	1.00	21.43
ATOM	1600	CG	HIS	259	14.019	14.066	10.746	1.00	18.22
ATOM	1601	CD2	HIS	259	15.287	14.145	10.278	1.00	24.02
ATOM	1602	ND1	HIS	259	13.946	12.882	11.446	1.00	16.87
ATOM	1603	CE1	HIS	259	15.114	12.273	11.405	1.00	22.04
ATOM	1604	NE2	HIS	259	15.947	13.017	10.703	1.00	20.47
ATOM	1605	C	HIS	259	10.438	15.366	11.158	1.00	22.70
ATOM	1606	O	HIS	259	10.588	16.154	12.093	1.00	25.27
ATOM	1607	N	LYS	260	9.369	15.367	10.368	1.00	17.40
ATOM	1608	CA	LYS	260	8.294	16.332	10.524	1.00	16.56
ATOM	1609	CB	LYS	260	8.265	17.268	9.312	1.00	19.39
ATOM	1610	CG	LYS	260	9.626	17.663	8.747	1.00	20.30
ATOM	1611	CD	LYS	260	9.443	18.546	7.519	1.00	28.30
ATOM	1612	CE	LYS	260	10.776	18.964	6.903	1.00	31.46
ATOM	1613	NZ	LYS	260	10.589	19.953	5.801	1.00	36.52
ATOM	1614	C	LYS	260	6.952	15.613	10.608	1.00	19.33
ATOM	1615	O	LYS	260	6.770	14.556	10.000	1.00	17.65
ATOM	1616	N	ILE	261	5.996	16.201	11.326	1.00	17.62
ATOM	1617	CA	ILE	261	4.668	15.602	11.449	1.00	14.19
ATOM	1618	CB	ILE	261	3.696	16.442	12.337	1.00	7.20
ATOM	1619	CG2	ILE	261	2.279	15.854	12.304	1.00	2.00
ATOM	1620	CG1	ILE	261	4.196	16.473	13.784	1.00	10.49
ATOM	1621	CD1	ILE	261	3.166	16.993	14.778	1.00	3.19
ATOM	1622	C	ILE	261	4.063	15.434	10.061	1.00	15.65
ATOM	1623	O	ILE	261	3.865	16.401	9.332	1.00	15.94
ATOM	1624	N	LEU	262	3.764	14.183	9.736	1.00	16.99
ATOM	1625	CA	LEU	262	3.193	13.773	8.460	1.00	16.61
ATOM	1626	CB	LEU	262	2.889	12.272	8.519	1.00	14.07
ATOM	1627	CG	LEU	262	3.555	11.337	7.510	1.00	11.45
ATOM	1628	CD1	LEU	262	5.061	11.292	7.728	1.00	7.82
ATOM	1629	CD2	LEU	262	2.931	9.958	7.638	1.00	3.94
ATOM	1630	C	LEU	262	1.930	14.541	8.025	1.00	19.12
ATOM	1631	O	LEU	262	1.886	15.071	6.909	1.00	20.84
ATOM	1632	N	PHE	263	0.909	14.571	8.877	1.00	19.61
ATOM	1633	CA	PHE	263	-0.344	15.263	8.556	1.00	19.23
ATOM	1634	CB	PHE	263	-1.498	14.264	8.419	1.00	20.11
ATOM	1635	CG	PHE	263	-1.123	12.991	7.714	1.00	31.62
ATOM	1636	CD1	PHE	263	-0.890	12.976	6.343	1.00	32.52
ATOM	1637	CD2	PHE	263	-1.007	11.800	8.425	1.00	32.72
ATOM	1638	CE1	PHE	263	-0.536	11.788	5.685	1.00	31.61
ATOM	1639	CE2	PHE	263	-0.655	10.606	7.784	1.00	31.76
ATOM	1640	CZ	PHE	263	-0.418	10.600	6.407	1.00	27.52
ATOM	1641	C	PHE	263	-0.714	16.277	9.643	1.00	21.98
ATOM	1642	O	PHE	263	-1.630	16.035	10.434	1.00	24.79
ATOM	1643	N	PRO	264	-0.020	17.428	9.690	1.00	22.78
ATOM	1644	CD	PRO	264	1.169	17.776	8.894	1.00	22.19
ATOM	1645	CA	PRO	264	-0.297	18.467	10.693	1.00	24.13
ATOM	1646	CB	PRO	264	1.035	19.210	10.774	1.00	21.59
ATOM	1647	CG	PRO	264	1.478	19.199	9.349	1.00	23.37
ATOM	1648	C	PRO	264	-1.456	19.396	10.319	1.00	24.33
ATOM	1649	O	PRO	264	-1.250	20.502	9.817	1.00	28.26
ATOM	1650	N	GLY	265	-2.674	18.939	10.587	1.00	23.20

FIG. 1CC

ATOM	1651	CA	GLY	265	-3.860	19.716	10.276	1.00	31.03
ATOM	1652	C	GLY	265	-4.302	20.680	11.361	1.00	37.14
ATOM	1653	O	GLY	265	-4.579	20.264	12.488	1.00	39.17
ATOM	1654	N	ARG	266	-4.404	21.961	11.007	1.00	39.70
ATOM	1655	CA	ARG	266	-4.816	23.013	11.933	1.00	38.28
ATOM	1656	CB	ARG	266	-4.703	24.374	11.255	1.00	40.99
ATOM	1657	CG	ARG	266	-3.263	24.775	10.975	1.00	47.16
ATOM	1658	CD	ARG	266	-3.171	26.160	10.337	1.00	50.47
ATOM	1659	NE	ARG	266	-2.047	26.921	10.877	1.00	52.30
ATOM	1660	CZ	ARG	266	-0.786	26.819	10.461	1.00	54.85
ATOM	1661	NH1	ARG	266	-0.462	25.988	9.476	1.00	54.82
ATOM	1662	NH2	ARG	266	0.165	27.528	11.061	1.00	55.46
ATOM	1663	C	ARG	266	-6.212	22.845	12.527	1.00	40.23
ATOM	1664	O	ARG	266	-6.500	23.392	13.594	1.00	42.31
ATOM	1665	N	ASP	267	-7.079	22.113	11.829	1.00	39.95
ATOM	1666	CA	ASP	267	-8.445	21.866	12.291	1.00	36.79
ATOM	1667	CB	ASP	267	-9.381	23.043	11.933	1.00	42.01
ATOM	1668	CG	ASP	267	-9.255	23.504	10.475	1.00	42.09
ATOM	1669	OD1	ASP	267	-10.263	23.420	9.734	1.00	37.79
ATOM	1670	OD2	ASP	267	-8.171	23.997	10.084	1.00	42.40
ATOM	1671	C	ASP	267	-8.989	20.531	11.776	1.00	34.35
ATOM	1672	O	ASP	267	-8.265	19.776	11.120	1.00	35.42
ATOM	1673	N	ALA	268	-10.257	20.245	12.073	1.00	31.62
ATOM	1674	CA	ALA	268	-10.903	18.999	11.659	1.00	30.64
ATOM	1675	CB	ALA	268	-12.337	18.955	12.188	1.00	28.57
ATOM	1676	C	ALA	268	-10.907	18.852	10.138	1.00	32.52
ATOM	1677	O	ALA	268	-10.762	17.746	9.599	1.00	28.70
ATOM	1678	N	ILE	269	-11.014	19.994	9.460	1.00	33.35
ATOM	1679	CA	ILE	269	-11.055	20.071	8.003	1.00	26.07
ATOM	1680	CB	ILE	269	-11.705	21.398	7.595	1.00	24.01
ATOM	1681	CG2	ILE	269	-11.614	21.610	6.087	1.00	24.76
ATOM	1682	CG1	ILE	269	-13.149	21.403	8.105	1.00	25.34
ATOM	1683	CD1	ILE	269	-13.785	22.763	8.199	1.00	20.60
ATOM	1684	C	ILE	269	-9.682	19.927	7.367	1.00	20.53
ATOM	1685	O	ILE	269	-9.492	19.133	6.459	1.00	20.91
ATOM	1686	N	ASP	270	-8.716	20.659	7.901	1.00	21.56
ATOM	1687	CA	ASP	270	-7.353	20.632	7.398	1.00	20.48
ATOM	1688	CB	ASP	270	-6.531	21.735	8.057	1.00	20.75
ATOM	1689	CG	ASP	270	-5.205	21.970	7.366	1.00	23.84
ATOM	1690	OD1	ASP	270	-5.172	21.986	6.113	1.00	28.48
ATOM	1691	OD2	ASP	270	-4.192	22.162	8.077	1.00	27.78
ATOM	1692	C	ASP	270	-6.685	19.290	7.640	1.00	23.87
ATOM	1693	O	ASP	270	-5.709	18.962	6.971	1.00	22.94
ATOM	1694	N	GLN	271	-7.185	18.524	8.610	1.00	27.87
ATOM	1695	CA	GLN	271	-6.611	17.213	8.917	1.00	26.15
ATOM	1696	CB	GLN	271	-7.225	16.634	10.200	1.00	29.33
ATOM	1697	CG	GLN	271	-6.560	15.344	10.683	1.00	30.10
ATOM	1698	CD	GLN	271	-5.054	15.469	10.774	1.00	33.24
ATOM	1699	OE1	GLN	271	-4.317	14.813	10.038	1.00	30.97
ATOM	1700	NE2	GLN	271	-4.588	16.345	11.655	1.00	36.55
ATOM	1701	C	GLN	271	-6.800	16.227	7.766	1.00	23.40
ATOM	1702	O	GLN	271	-5.843	15.587	7.330	1.00	17.83
ATOM	1703	N	TRP	272	-8.032	16.126	7.270	1.00	21.41
ATOM	1704	CA	TRP	272	-8.352	15.221	6.174	1.00	21.27
ATOM	1705	CB	TRP	272	-9.862	15.184	5.944	1.00	25.91
ATOM	1706	CG	TRP	272	-10.320	14.231	4.855	1.00	34.96
ATOM	1707	CD2	TRP	272	-10.216	12.790	4.856	1.00	37.63
ATOM	1708	CE2	TRP	272	-10.864	12.322	3.684	1.00	39.04
ATOM	1709	CE3	TRP	272	-9.645	11.857	5.733	1.00	36.23

FIG. 1DD

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ATOM   1710  CD1 TRP   272     -11.001  14.559   3.706  1.00  34.40
ATOM   1711  NE1 TRP   272     -11.333  13.420   3.004  1.00  34.42
ATOM   1712  CZ2 TRP   272     -10.954  10.956   3.373  1.00  38.88
ATOM   1713  CZ3 TRP   272      -9.733  10.504   5.427  1.00  33.36
ATOM   1714  CH2 TRP   272     -10.385  10.063   4.257  1.00  37.17
ATOM   1715  C   TRP   272      -7.647  15.626   4.887  1.00  23.52
ATOM   1716  O   TRP   272      -7.130  14.774   4.165  1.00  25.26
ATOM   1717  N   ASN   273      -7.576  16.930   4.632  1.00  24.61
ATOM   1718  CA  ASN   273      -6.947  17.449   3.424  1.00  20.66
ATOM   1719  CB  ASN   273      -7.186  18.954   3.290  1.00  22.38
ATOM   1720  CG  ASN   273      -8.625  19.285   2.939  1.00  22.57
ATOM   1721  OD1 ASN   273      -9.275  18.551   2.192  1.00  16.68
ATOM   1722  ND2 ASN   273      -9.135  20.389   3.480  1.00  19.51
ATOM   1723  C   ASN   273      -5.469  17.158   3.394  1.00  18.46
ATOM   1724  O   ASN   273      -4.893  16.944   2.326  1.00  24.72
ATOM   1725  N   LYS   274      -4.849  17.153   4.565  1.00  17.40
ATOM   1726  CA  LYS   274      -3.423  16.863   4.681  1.00  20.54
ATOM   1727  CB  LYS   274      -2.946  17.126   6.117  1.00  24.00
ATOM   1728  CG  LYS   274      -2.820  18.606   6.490  1.00  23.91
ATOM   1729  CD  LYS   274      -1.570  19.229   5.890  1.00  31.69
ATOM   1730  CE  LYS   274      -1.429  20.711   6.242  1.00  36.12
ATOM   1731  NZ  LYS   274      -2.396  21.581   5.504  1.00  39.86
ATOM   1732  C   LYS   274      -3.170  15.401   4.301  1.00  19.94
ATOM   1733  O   LYS   274      -2.091  15.056   3.815  1.00  17.57
ATOM   1734  N   VAL   275      -4.188  14.561   4.500  1.00  21.20
ATOM   1735  CA  VAL   275      -4.135  13.129   4.195  1.00  21.22
ATOM   1736  CB  VAL   275      -5.260  12.356   4.947  1.00  27.34
ATOM   1737  CG1 VAL   275      -5.249  10.863   4.570  1.00  24.55
ATOM   1738  CG2 VAL   275      -5.100  12.535   6.450  1.00  21.86
ATOM   1739  C   VAL   275      -4.246  12.822   2.695  1.00  19.42
ATOM   1740  O   VAL   275      -3.321  12.258   2.105  1.00  19.86
ATOM   1741  N   ILE   276      -5.368  13.195   2.078  1.00  15.37
ATOM   1742  CA  ILE   276      -5.561  12.949   0.655  1.00  10.70
ATOM   1743  CB  ILE   276      -7.020  13.177   0.217  1.00   2.68
ATOM   1744  CG2 ILE   276      -7.948  12.312   1.052  1.00   2.00
ATOM   1745  CG1 ILE   276      -7.393  14.642   0.337  1.00   2.00
ATOM   1746  CD1 ILE   276      -8.879  14.892   0.120  1.00   2.00
ATOM   1747  C   ILE   276      -4.608  13.728  -0.244  1.00  11.53
ATOM   1748  O   ILE   276      -4.358  13.332  -1.378  1.00  13.01
ATOM   1749  N   GLU   277      -4.034  14.810   0.258  1.00  17.68
ATOM   1750  CA  GLU   277      -3.085  15.574  -0.546  1.00  21.93
ATOM   1751  CB  GLU   277      -2.609  16.805   0.228  1.00  26.73
ATOM   1752  CG  GLU   277      -3.333  18.094  -0.107  1.00  31.15
ATOM   1753  CD  GLU   277      -3.082  19.186   0.920  1.00  31.05
ATOM   1754  OE1 GLU   277      -1.907  19.418   1.278  1.00  28.67
ATOM   1755  OE2 GLU   277      -4.066  19.805   1.378  1.00  30.92
ATOM   1756  C   GLU   277      -1.879  14.694  -0.874  1.00  23.55
ATOM   1757  O   GLU   277      -1.367  14.704  -2.002  1.00  25.88
ATOM   1758  N   GLN   278      -1.471  13.895   0.111  1.00  20.15
ATOM   1759  CA  GLN   278      -0.310  13.018  -0.002  1.00  17.85
ATOM   1760  CB  GLN   278       0.412  12.945   1.335  1.00  15.48
ATOM   1761  CG  GLN   278       0.945  14.239   1.858  1.00  13.04
ATOM   1762  CD  GLN   278       1.552  14.053   3.223  1.00   9.75
ATOM   1763  OE1 GLN   278       2.682  13.588   3.359  1.00   9.48
ATOM   1764  NE2 GLN   278       0.796  14.397   4.246  1.00  12.91
ATOM   1765  C   GLN   278      -0.591  11.592  -0.435  1.00  15.71
ATOM   1766  O   GLN   278       0.260  10.959  -1.055  1.00  16.36
ATOM   1767  N   LEU   279      -1.753  11.078  -0.055  1.00  11.53
ATOM   1768  CA  LEU   279      -2.115   9.711  -0.367  1.00  12.00
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FIG. 1EE

ATOM	1769	CB	LEU	279	-2.639	9.017	0.887	1.00	12.00
ATOM	1770	CG	LEU	279	-1.786	9.084	2.158	1.00	9.51
ATOM	1771	CD1	LEU	279	-2.339	8.079	3.146	1.00	6.61
ATOM	1772	CD2	LEU	279	-0.315	8.805	1.867	1.00	3.14
ATOM	1773	C	LEU	279	-3.124	9.578	-1.500	1.00	17.06
ATOM	1774	O	LEU	279	-3.161	8.562	-2.198	1.00	18.67
ATOM	1775	N	GLY	280	-3.926	10.613	-1.696	1.00	18.66
ATOM	1776	CA	GLY	280	-4.909	10.587	-2.757	1.00	15.54
ATOM	1777	C	GLY	280	-6.307	10.343	-2.251	1.00	16.01
ATOM	1778	O	GLY	280	-6.505	9.822	-1.153	1.00	18.83
ATOM	1779	N	THR	281	-7.287	10.740	-3.045	1.00	17.90
ATOM	1780	CA	THR	281	-8.676	10.558	-2.678	1.00	20.47
ATOM	1781	CB	THR	281	-9.603	11.349	-3.622	1.00	16.28
ATOM	1782	OG1	THR	281	-9.144	12.706	-3.706	1.00	17.45
ATOM	1783	CG2	THR	281	-11.037	11.351	-3.112	1.00	17.34
ATOM	1784	C	THR	281	-8.975	9.062	-2.748	1.00	26.86
ATOM	1785	O	THR	281	-8.603	8.394	-3.712	1.00	31.52
ATOM	1786	N	PRO	282	-9.563	8.511	-1.680	1.00	28.38
ATOM	1787	CD	PRO	282	-9.854	9.208	-0.418	1.00	25.29
ATOM	1788	CA	PRO	282	-9.919	7.092	-1.573	1.00	26.47
ATOM	1789	CB	PRO	282	-10.421	6.980	-0.136	1.00	21.64
ATOM	1790	CG	PRO	282	-10.959	8.351	0.155	1.00	21.02
ATOM	1791	C	PRO	282	-10.960	6.570	-2.560	1.00	25.85
ATOM	1792	O	PRO	282	-11.840	7.299	-3.022	1.00	25.44
ATOM	1793	N	CYS	283	-10.855	5.269	-2.822	1.00	25.32
ATOM	1794	CA	CYS	283	-11.722	4.532	-3.729	1.00	24.18
ATOM	1795	CB	CYS	283	-11.255	3.071	-3.797	1.00	26.45
ATOM	1796	SG	CYS	283	-11.206	2.192	-2.201	1.00	38.53
ATOM	1797	C	CYS	283	-13.171	4.600	-3.285	1.00	20.79
ATOM	1798	O	CYS	283	-13.449	4.791	-2.113	1.00	25.27
ATOM	1799	N	PRO	284	-14.117	4.474	-4.231	1.00	21.61
ATOM	1800	CD	PRO	284	-13.890	4.378	-5.686	1.00	17.56
ATOM	1801	CA	PRO	284	-15.555	4.515	-3.926	1.00	18.26
ATOM	1802	CB	PRO	284	-16.199	4.309	-5.299	1.00	20.65
ATOM	1803	CG	PRO	284	-15.185	4.905	-6.246	1.00	17.52
ATOM	1804	C	PRO	284	-15.974	3.424	-2.943	1.00	19.06
ATOM	1805	O	PRO	284	-17.050	3.483	-2.358	1.00	20.50
ATOM	1806	N	ALA	285	-15.126	2.411	-2.788	1.00	21.71
ATOM	1807	CA	ALA	285	-15.394	1.310	-1.878	1.00	26.28
ATOM	1808	CB	ALA	285	-14.325	0.234	-2.043	1.00	26.44
ATOM	1809	C	ALA	285	-15.393	1.848	-0.446	1.00	27.71
ATOM	1810	O	ALA	285	-16.212	1.451	0.388	1.00	29.33
ATOM	1811	N	PHE	286	-14.462	2.763	-0.193	1.00	27.78
ATOM	1812	CA	PHE	286	-14.289	3.409	1.098	1.00	23.59
ATOM	1813	CB	PHE	286	-12.940	4.118	1.097	1.00	24.13
ATOM	1814	CG	PHE	286	-12.628	4.831	2.373	1.00	29.65
ATOM	1815	CD1	PHE	286	-12.212	4.123	3.494	1.00	31.45
ATOM	1816	CD2	PHE	286	-12.702	6.216	2.439	1.00	31.48
ATOM	1817	CE1	PHE	286	-11.874	4.786	4.664	1.00	32.34
ATOM	1818	CE2	PHE	286	-12.368	6.891	3.598	1.00	32.31
ATOM	1819	CZ	PHE	286	-11.949	6.175	4.716	1.00	32.68
ATOM	1820	C	PHE	286	-15.401	4.425	1.284	1.00	22.60
ATOM	1821	O	PHE	286	-16.135	4.391	2.270	1.00	25.95
ATOM	1822	N	MET	287	-15.561	5.291	0.288	1.00	19.48
ATOM	1823	CA	MET	287	-16.570	6.332	0.311	1.00	16.74
ATOM	1824	CB	MET	287	-16.580	7.106	-1.017	1.00	18.72
ATOM	1825	CG	MET	287	-15.314	7.938	-1.283	1.00	20.14
ATOM	1826	SD	MET	287	-14.974	9.280	-0.078	1.00	20.20
ATOM	1827	CE	MET	287	-13.753	10.219	-0.961	1.00	24.44

FIG. 1FF

ATOM	1828	C	MET	287	-17.955	5.782	0.625	1.00	16.03
ATOM	1829	O	MET	287	-18.659	6.331	1.456	1.00	18.99
ATOM	1830	N	ALA	288	-18.317	4.662	0.013	1.00	20.90
ATOM	1831	CA	ALA	288	-19.626	4.066	0.236	1.00	26.22
ATOM	1832	CB	ALA	288	-19.826	2.875	-0.694	1.00	26.60
ATOM	1833	C	ALA	288	-19.833	3.653	1.693	1.00	28.97
ATOM	1834	O	ALA	288	-20.966	3.584	2.165	1.00	31.30
ATOM	1835	N	LYS	289	-18.742	3.380	2.407	1.00	32.21
ATOM	1836	CA	LYS	289	-18.829	2.993	3.815	1.00	33.61
ATOM	1837	CB	LYS	289	-17.500	2.391	4.301	1.00	34.28
ATOM	1838	CG	LYS	289	-17.428	0.858	4.209	1.00	34.62
ATOM	1839	CD	LYS	289	-18.440	0.200	5.149	1.00	37.66
ATOM	1840	CE	LYS	289	-18.111	0.495	6.622	1.00	37.54
ATOM	1841	NZ	LYS	289	-19.268	0.291	7.549	1.00	34.87
ATOM	1842	C	LYS	289	-19.230	4.193	4.676	1.00	33.97
ATOM	1843	O	LYS	289	-19.769	4.039	5.775	1.00	33.49
ATOM	1844	N	LEU	290	-18.988	5.388	4.147	1.00	35.80
ATOM	1845	CA	LEU	290	-19.327	6.637	4.827	1.00	35.58
ATOM	1846	CB	LEU	290	-18.652	7.820	4.134	1.00	31.46
ATOM	1847	CG	LEU	290	-17.135	7.854	4.011	1.00	30.05
ATOM	1848	CD1	LEU	290	-16.721	8.881	2.970	1.00	29.96
ATOM	1849	CD2	LEU	290	-16.530	8.166	5.353	1.00	34.22
ATOM	1850	C	LEU	290	-20.831	6.874	4.759	1.00	37.04
ATOM	1851	O	LEU	290	-21.452	6.666	3.719	1.00	39.41
ATOM	1852	N	GLN	291	-21.423	7.317	5.862	1.00	40.14
ATOM	1853	CA	GLN	291	-22.846	7.610	5.849	1.00	41.39
ATOM	1854	CB	GLN	291	-23.442	7.657	7.268	1.00	42.50
ATOM	1855	CG	GLN	291	-22.524	8.174	8.362	1.00	45.42
ATOM	1856	CD	GLN	291	-22.640	7.367	9.650	1.00	48.95
ATOM	1857	OE1	GLN	291	-21.630	7.009	10.265	1.00	48.41
ATOM	1858	NE2	GLN	291	-23.871	7.039	10.042	1.00	46.58
ATOM	1859	C	GLN	291	-23.028	8.927	5.091	1.00	41.36
ATOM	1860	O	GLN	291	-22.238	9.856	5.243	1.00	37.77
ATOM	1861	N	PRO	292	-24.047	8.990	4.221	1.00	42.77
ATOM	1862	CD	PRO	292	-25.090	7.948	4.215	1.00	43.22
ATOM	1863	CA	PRO	292	-24.454	10.101	3.360	1.00	40.98
ATOM	1864	CB	PRO	292	-25.969	10.063	3.500	1.00	42.32
ATOM	1865	CG	PRO	292	-26.226	8.589	3.401	1.00	41.51
ATOM	1866	C	PRO	292	-23.866	11.475	3.662	1.00	38.85
ATOM	1867	O	PRO	292	-23.138	12.025	2.835	1.00	37.72
ATOM	1868	N	THR	293	-24.146	11.998	4.853	1.00	36.06
ATOM	1869	CA	THR	293	-23.667	13.319	5.263	1.00	30.91
ATOM	1870	CB	THR	293	-24.095	13.640	6.709	1.00	35.11
ATOM	1871	OG1	THR	293	-25.513	13.472	6.841	1.00	37.56
ATOM	1872	CG2	THR	293	-23.701	15.076	7.083	1.00	37.03
ATOM	1873	C	THR	293	-22.151	13.401	5.207	1.00	27.49
ATOM	1874	O	THR	293	-21.587	14.384	4.727	1.00	27.10
ATOM	1875	N	VAL	294	-21.496	12.382	5.749	1.00	26.19
ATOM	1876	CA	VAL	294	-20.046	12.320	5.770	1.00	23.72
ATOM	1877	CB	VAL	294	-19.549	11.159	6.675	1.00	19.37
ATOM	1878	CG1	VAL	294	-18.045	11.238	6.874	1.00	13.70
ATOM	1879	CG2	VAL	294	-20.263	11.189	8.010	1.00	15.03
ATOM	1880	C	VAL	294	-19.553	12.099	4.345	1.00	29.48
ATOM	1881	O	VAL	294	-18.493	12.609	3.955	1.00	33.31
ATOM	1882	N	ARG	295	-20.336	11.368	3.554	1.00	31.18
ATOM	1883	CA	ARG	295	-19.958	11.104	2.169	1.00	30.61
ATOM	1884	CB	ARG	295	-20.976	10.186	1.480	1.00	32.61
ATOM	1885	CG	ARG	295	-20.355	9.204	0.472	1.00	33.15
ATOM	1886	CD	ARG	295	-21.376	8.819	-0.609	1.00	41.22

FIG. 1GG

ATOM	1887	NE	ARG	295	-21.116	7.549	-1.303	1.00	44.77
ATOM	1888	CZ	ARG	295	-20.157	7.332	-2.206	1.00	45.75
ATOM	1889	NH1	ARG	295	-19.314	8.289	-2.560	1.00	42.66
ATOM	1890	NH2	ARG	295	-20.077	6.153	-2.808	1.00	50.09
ATOM	1891	C	ARG	295	-19.893	12.458	1.461	1.00	26.05
ATOM	1892	O	ARG	295	-18.879	12.794	0.855	1.00	27.82
ATOM	1893	N	ASN	296	-20.929	13.272	1.655	1.00	25.63
ATOM	1894	CA	ASN	296	-21.011	14.600	1.048	1.00	23.53
ATOM	1895	CB	ASN	296	-22.313	15.305	1.446	1.00	24.22
ATOM	1896	CG	ASN	296	-23.551	14.648	0.858	1.00	28.67
ATOM	1897	OD1	ASN	296	-23.496	13.529	0.347	1.00	36.26
ATOM	1898	ND2	ASN	296	-24.684	15.345	0.928	1.00	30.43
ATOM	1899	C	ASN	296	-19.829	15.470	1.456	1.00	24.99
ATOM	1900	O	ASN	296	-19.059	15.913	0.605	1.00	26.73
ATOM	1901	N	TYR	297	-19.655	15.661	2.762	1.00	26.38
ATOM	1902	CA	TYR	297	-18.582	16.488	3.311	1.00	26.13
ATOM	1903	CB	TYR	297	-18.594	16.387	4.847	1.00	32.32
ATOM	1904	CG	TYR	297	-17.278	16.685	5.538	1.00	32.85
ATOM	1905	CD1	TYR	297	-16.755	17.972	5.580	1.00	32.13
ATOM	1906	CE1	TYR	297	-15.533	18.229	6.202	1.00	34.78
ATOM	1907	CD2	TYR	297	-16.549	15.666	6.139	1.00	34.34
ATOM	1908	CE2	TYR	297	-15.331	15.917	6.758	1.00	36.24
ATOM	1909	CZ	TYR	297	-14.829	17.194	6.785	1.00	34.88
ATOM	1910	OH	TYR	297	-13.613	17.422	7.386	1.00	40.94
ATOM	1911	C	TYR	297	-17.198	16.169	2.746	1.00	23.94
ATOM	1912	O	TYR	297	-16.405	17.077	2.484	1.00	16.61
ATOM	1913	N	VAL	298	-16.936	14.879	2.547	1.00	26.14
ATOM	1914	CA	VAL	298	-15.665	14.381	2.026	1.00	24.39
ATOM	1915	CB	VAL	298	-15.394	12.936	2.541	1.00	22.80
ATOM	1916	CG1	VAL	298	-14.102	12.362	1.941	1.00	19.07
ATOM	1917	CG2	VAL	298	-15.302	12.942	4.054	1.00	19.85
ATOM	1918	C	VAL	298	-15.573	14.411	0.497	1.00	25.08
ATOM	1919	O	VAL	298	-14.478	14.520	-0.065	1.00	26.44
ATOM	1920	N	GLU	299	-16.713	14.330	-0.179	1.00	27.22
ATOM	1921	CA	GLU	299	-16.727	14.360	-1.635	1.00	27.74
ATOM	1922	CB	GLU	299	-18.052	13.849	-2.170	1.00	28.52
ATOM	1923	CG	GLU	299	-17.887	12.975	-3.380	1.00	33.99
ATOM	1924	CD	GLU	299	-17.578	11.548	-3.000	1.00	28.84
ATOM	1925	OE1	GLU	299	-18.536	10.810	-2.703	1.00	21.31
ATOM	1926	OE2	GLU	299	-16.391	11.164	-2.994	1.00	26.35
ATOM	1927	C	GLU	299	-16.509	15.775	-2.155	1.00	26.19
ATOM	1928	O	GLU	299	-15.767	15.974	-3.113	1.00	27.10
ATOM	1929	N	ASN	300	-17.175	16.749	-1.534	1.00	24.87
ATOM	1930	CA	ASN	300	-17.063	18.148	-1.937	1.00	20.43
ATOM	1931	CB	ASN	300	-18.163	18.979	-1.273	1.00	20.76
ATOM	1932	CG	ASN	300	-18.468	20.260	-2.031	1.00	25.51
ATOM	1933	OD1	ASN	300	-17.629	20.784	-2.765	1.00	29.81
ATOM	1934	ND2	ASN	300	-19.684	20.768	-1.863	1.00	29.41
ATOM	1935	C	ASN	300	-15.692	18.645	-1.509	1.00	17.56
ATOM	1936	O	ASN	300	-15.553	19.325	-0.500	1.00	21.18
ATOM	1937	N	ARG	301	-14.684	18.282	-2.287	1.00	18.56
ATOM	1938	CA	ARG	301	-13.296	18.637	-2.022	1.00	20.80
ATOM	1939	CB	ARG	301	-12.733	17.754	-0.902	1.00	27.14
ATOM	1940	CG	ARG	301	-12.739	18.365	0.486	1.00	31.25
ATOM	1941	CD	ARG	301	-12.089	17.398	1.454	1.00	30.07
ATOM	1942	NE	ARG	301	-11.876	17.989	2.766	1.00	35.05
ATOM	1943	CZ	ARG	301	-12.796	18.034	3.721	1.00	39.13
ATOM	1944	NH1	ARG	301	-14.000	17.516	3.513	1.00	34.08
ATOM	1945	NH2	ARG	301	-12.507	18.601	4.888	1.00	42.53

FIG. 1HH

ATOM	1946	C	ARG	301	-12.518	18.332	-3.287	1.00	20.56
ATOM	1947	O	ARG	301	-12.956	17.539	-4.101	1.00	23.26
ATOM	1948	N	PRO	302	-11.349	18.948	-3.464	1.00	21.89
ATOM	1949	CD	PRO	302	-10.670	19.941	-2.619	1.00	25.17
ATOM	1950	CA	PRO	302	-10.572	18.668	-4.670	1.00	25.44
ATOM	1951	CB	PRO	302	-9.407	19.651	-4.559	1.00	26.64
ATOM	1952	CG	PRO	302	-9.236	19.813	-3.084	1.00	24.33
ATOM	1953	C	PRO	302	-10.086	17.228	-4.661	1.00	29.44
ATOM	1954	O	PRO	302	-9.595	16.750	-3.637	1.00	34.61
ATOM	1955	N	LYS	303	-10.274	16.531	-5.784	1.00	28.85
ATOM	1956	CA	LYS	303	-9.857	15.145	-5.927	1.00	21.63
ATOM	1957	CB	LYS	303	-10.662	14.449	-7.034	1.00	24.46
ATOM	1958	CG	LYS	303	-10.849	15.266	-8.323	1.00	41.84
ATOM	1959	CD	LYS	303	-11.871	14.622	-9.290	1.00	44.46
ATOM	1960	CE	LYS	303	-12.064	15.458	-10.568	1.00	45.69
ATOM	1961	NZ	LYS	303	-13.119	14.930	-11.491	1.00	45.06
ATOM	1962	C	LYS	303	-8.358	15.096	-6.189	1.00	20.81
ATOM	1963	O	LYS	303	-7.807	15.966	-6.858	1.00	20.42
ATOM	1964	N	TYR	304	-7.685	14.130	-5.571	1.00	21.39
ATOM	1965	CA	TYR	304	-6.240	13.971	-5.710	1.00	21.82
ATOM	1966	CB	TYR	304	-5.534	14.211	-4.368	1.00	24.87
ATOM	1967	CG	TYR	304	-5.666	15.594	-3.807	1.00	23.11
ATOM	1968	CD1	TYR	304	-6.777	15.959	-3.050	1.00	23.67
ATOM	1969	CE1	TYR	304	-6.900	17.244	-2.517	1.00	20.86
ATOM	1970	CD2	TYR	304	-4.677	16.545	-4.017	1.00	26.39
ATOM	1971	CE2	TYR	304	-4.795	17.833	-3.486	1.00	24.30
ATOM	1972	CZ	TYR	304	-5.907	18.171	-2.742	1.00	23.26
ATOM	1973	OH	TYR	304	-6.032	19.447	-2.251	1.00	28.31
ATOM	1974	C	TYR	304	-5.891	12.563	-6.151	1.00	21.83
ATOM	1975	O	TYR	304	-6.662	11.623	-5.959	1.00	21.88
ATOM	1976	N	ALA	305	-4.714	12.429	-6.750	1.00	23.94
ATOM	1977	CA	ALA	305	-4.221	11.128	-7.189	1.00	27.30
ATOM	1978	CB	ALA	305	-3.483	11.259	-8.516	1.00	22.41
ATOM	1979	C	ALA	305	-3.270	10.651	-6.106	1.00	25.62
ATOM	1980	O	ALA	305	-3.089	9.455	-5.893	1.00	28.28
ATOM	1981	N	GLY	306	-2.641	11.617	-5.441	1.00	23.97
ATOM	1982	CA	GLY	306	-1.714	11.321	-4.366	1.00	21.65
ATOM	1983	C	GLY	306	-0.381	10.870	-4.891	1.00	19.70
ATOM	1984	O	GLY	306	-0.316	10.093	-5.837	1.00	21.53
ATOM	1985	N	LEU	307	0.686	11.344	-4.266	1.00	18.69
ATOM	1986	CA	LEU	307	2.036	10.987	-4.688	1.00	18.55
ATOM	1987	CB	LEU	307	3.071	11.862	-3.984	1.00	15.42
ATOM	1988	CG	LEU	307	2.718	13.327	-3.740	1.00	15.82
ATOM	1989	CD1	LEU	307	3.925	14.060	-3.185	1.00	9.35
ATOM	1990	CD2	LEU	307	2.258	13.958	-5.034	1.00	20.09
ATOM	1991	C	LEU	307	2.346	9.530	-4.390	1.00	22.25
ATOM	1992	O	LEU	307	1.692	8.885	-3.565	1.00	27.73
ATOM	1993	N	THR	308	3.328	9.000	-5.104	1.00	24.37
ATOM	1994	CA	THR	308	3.758	7.629	-4.892	1.00	23.85
ATOM	1995	CB	THR	308	4.552	7.102	-6.105	1.00	26.19
ATOM	1996	OG1	THR	308	5.662	7.969	-6.375	1.00	25.39
ATOM	1997	CG2	THR	308	3.654	7.031	-7.333	1.00	26.29
ATOM	1998	C	THR	308	4.661	7.688	-3.659	1.00	21.47
ATOM	1999	O	THR	308	5.242	8.729	-3.368	1.00	24.53
ATOM	2000	N	PHE	309	4.806	6.576	-2.954	1.00	16.71
ATOM	2001	CA	PHE	309	5.628	6.552	-1.759	1.00	12.56
ATOM	2002	CB	PHE	309	5.510	5.229	-1.032	1.00	13.01
ATOM	2003	CG	PHE	309	4.279	5.139	-0.212	1.00	2.00
ATOM	2004	CD1	PHE	309	3.052	4.935	-0.821	1.00	2.00

FIG. 1II

ATOM	2005	CD2	PHE	309	4.328	5.363	1.152	1.00	3.00
ATOM	2006	CE1	PHE	309	1.875	4.957	-0.089	1.00	2.72
ATOM	2007	CE2	PHE	309	3.161	5.391	1.904	1.00	2.24
ATOM	2008	CZ	PHE	309	1.925	5.187	1.281	1.00	2.00
ATOM	2009	C	PHE	309	7.063	6.949	-1.942	1.00	14.67
ATOM	2010	O	PHE	309	7.671	7.453	-1.003	1.00	21.23
ATOM	2011	N	PRO	310	7.658	6.661	-3.102	1.00	16.62
ATOM	2012	CD	PRO	310	7.386	5.631	-4.133	1.00	15.13
ATOM	2013	CA	PRO	310	9.053	7.110	-3.158	1.00	13.22
ATOM	2014	CB	PRO	310	9.676	6.241	-4.256	1.00	12.65
ATOM	2015	CG	PRO	310	8.523	5.838	-5.108	1.00	7.98
ATOM	2016	C	PRO	310	9.143	8.630	-3.382	1.00	13.94
ATOM	2017	O	PRO	310	10.226	9.216	-3.317	1.00	16.27
ATOM	2018	N	LYS	311	7.996	9.257	-3.628	1.00	15.44
ATOM	2019	CA	LYS	311	7.935	10.708	-3.781	1.00	15.60
ATOM	2020	CB	LYS	311	6.795	11.132	-4.707	1.00	17.57
ATOM	2021	CG	LYS	311	7.044	10.862	-6.190	1.00	26.47
ATOM	2022	CD	LYS	311	8.243	11.638	-6.731	1.00	31.84
ATOM	2023	CE	LYS	311	8.438	11.399	-8.232	1.00	36.14
ATOM	2024	NZ	LYS	311	9.587	12.165	-8.813	1.00	36.37
ATOM	2025	C	LYS	311	7.681	11.225	-2.363	1.00	18.67
ATOM	2026	O	LYS	311	8.301	12.192	-1.925	1.00	21.81
ATOM	2027	N	LEU	312	6.793	10.534	-1.641	1.00	18.78
ATOM	2028	CA	LEU	312	6.451	10.864	-0.254	1.00	13.83
ATOM	2029	CB	LEU	312	5.289	10.003	0.240	1.00	2.00
ATOM	2030	CG	LEU	312	3.891	10.286	-0.301	1.00	2.00
ATOM	2031	CD1	LEU	312	2.882	9.395	0.370	1.00	2.00
ATOM	2032	CD2	LEU	312	3.540	11.718	-0.037	1.00	3.52
ATOM	2033	C	LEU	312	7.655	10.637	0.667	1.00	15.47
ATOM	2034	O	LEU	312	7.805	11.348	1.666	1.00	19.46
ATOM	2035	N	PHE	313	8.491	9.656	0.329	1.00	13.49
ATOM	2036	CA	PHE	313	9.683	9.326	1.118	1.00	14.43
ATOM	2037	CB	PHE	313	9.434	8.124	2.047	1.00	10.04
ATOM	2038	CG	PHE	313	8.287	8.327	2.997	1.00	7.55
ATOM	2039	CD1	PHE	313	7.020	7.843	2.679	1.00	4.93
ATOM	2040	CD2	PHE	313	8.458	9.044	4.179	1.00	2.84
ATOM	2041	CE1	PHE	313	5.920	8.074	3.505	1.00	2.00
ATOM	2042	CE2	PHE	313	7.376	9.288	5.021	1.00	2.00
ATOM	2043	CZ	PHE	313	6.094	8.803	4.684	1.00	4.98
ATOM	2044	C	PHE	313	10.896	9.045	0.234	1.00	15.60
ATOM	2045	O	PHE	313	11.217	7.897	-0.056	1.00	23.18
ATOM	2046	N	PRO	314	11.573	10.102	-0.217	1.00	14.26
ATOM	2047	CD	PRO	314	11.109	11.483	-0.006	1.00	17.51
ATOM	2048	CA	PRO	314	12.763	10.085	-1.067	1.00	17.53
ATOM	2049	CB	PRO	314	13.096	11.578	-1.210	1.00	15.23
ATOM	2050	CG	PRO	314	11.767	12.228	-1.149	1.00	13.83
ATOM	2051	C	PRO	314	13.937	9.357	-0.429	1.00	19.49
ATOM	2052	O	PRO	314	14.018	9.240	0.792	1.00	20.42
ATOM	2053	N	ASP	315	14.877	8.924	-1.266	1.00	22.24
ATOM	2054	CA	ASP	315	16.082	8.238	-0.807	1.00	27.08
ATOM	2055	CB	ASP	315	16.718	7.447	-1.958	1.00	36.01
ATOM	2056	CG	ASP	315	16.063	6.099	-2.174	1.00	40.69
ATOM	2057	OD1	ASP	315	15.166	6.006	-3.041	1.00	45.06
ATOM	2058	OD2	ASP	315	16.449	5.132	-1.474	1.00	47.14
ATOM	2059	C	ASP	315	17.099	9.216	-0.217	1.00	25.78
ATOM	2060	O	ASP	315	18.221	8.831	0.139	1.00	27.53
ATOM	2061	N	SER	316	16.736	10.496	-0.204	1.00	23.63
ATOM	2062	CA	SER	316	17.583	11.540	0.359	1.00	20.13
ATOM	2063	CB	SER	316	17.239	12.896	-0.255	1.00	16.00

FIG. 1JJ

ATOM	2064	OG	SER	316	15.835	13.079	-0.336	1.00	14.43
ATOM	2065	C	SER	316	17.360	11.549	1.866	1.00	16.95
ATOM	2066	O	SER	316	18.211	11.999	2.625	1.00	19.02
ATOM	2067	N	LEU	317	16.191	11.062	2.273	1.00	11.69
ATOM	2068	CA	LEU	317	15.827	10.956	3.671	1.00	10.42
ATOM	2069	CB	LEU	317	14.329	10.732	3.816	1.00	6.04
ATOM	2070	CG	LEU	317	13.428	11.848	3.325	1.00	7.50
ATOM	2071	CD1	LEU	317	11.977	11.478	3.602	1.00	2.00
ATOM	2072	CD2	LEU	317	13.826	13.131	4.033	1.00	9.21
ATOM	2073	C	LEU	317	16.546	9.771	4.306	1.00	14.46
ATOM	2074	O	LEU	317	17.018	9.876	5.432	1.00	22.75
ATOM	2075	N	PHE	318	16.581	8.643	3.596	1.00	14.45
ATOM	2076	CA	PHE	318	17.224	7.424	4.083	1.00	10.89
ATOM	2077	CB	PHE	318	16.590	6.191	3.452	1.00	6.43
ATOM	2078	CG	PHE	318	15.095	6.168	3.504	1.00	2.63
ATOM	2079	CD1	PHE	318	14.351	6.728	2.482	1.00	2.00
ATOM	2080	CD2	PHE	318	14.431	5.531	4.544	1.00	7.53
ATOM	2081	CE1	PHE	318	12.958	6.658	2.479	1.00	2.00
ATOM	2082	CE2	PHE	318	13.034	5.450	4.561	1.00	6.05
ATOM	2083	CZ	PHE	318	12.294	6.017	3.517	1.00	3.68
ATOM	2084	C	PHE	318	18.689	7.388	3.700	1.00	15.81
ATOM	2085	O	PHE	318	19.110	8.087	2.789	1.00	24.20
ATOM	2086	N	PRO	319	19.505	6.625	4.443	1.00	17.34
ATOM	2087	CD	PRO	319	19.258	6.115	5.805	1.00	13.79
ATOM	2088	CA	PRO	319	20.931	6.546	4.089	1.00	20.27
ATOM	2089	CB	PRO	319	21.579	6.029	5.378	1.00	19.75
ATOM	2090	CG	PRO	319	20.472	5.258	6.058	1.00	15.80
ATOM	2091	C	PRO	319	21.077	5.556	2.913	1.00	24.31
ATOM	2092	O	PRO	319	20.155	4.782	2.648	1.00	21.99
ATOM	2093	N	ALA	320	22.196	5.599	2.185	1.00	26.79
ATOM	2094	CA	ALA	320	22.375	4.695	1.045	1.00	27.80
ATOM	2095	CB	ALA	320	21.552	5.183	-0.148	1.00	27.57
ATOM	2096	C	ALA	320	23.818	4.473	0.620	1.00	29.97
ATOM	2097	O	ALA	320	24.100	4.274	-0.561	1.00	25.49
ATOM	2098	N	ASP	321	24.738	4.488	1.575	1.00	34.44
ATOM	2099	CA	ASP	321	26.145	4.267	1.246	1.00	38.90
ATOM	2100	CB	ASP	321	27.056	4.965	2.269	1.00	42.26
ATOM	2101	CG	ASP	321	26.867	4.424	3.672	1.00	48.36
ATOM	2102	OD1	ASP	321	25.821	4.724	4.293	1.00	50.98
ATOM	2103	OD2	ASP	321	27.759	3.683	4.144	1.00	52.03
ATOM	2104	C	ASP	321	26.445	2.757	1.195	1.00	37.24
ATOM	2105	O	ASP	321	27.601	2.337	1.349	1.00	36.84
ATOM	2106	N	SER	322	25.404	1.951	0.994	1.00	28.45
ATOM	2107	CA	SER	322	25.560	0.504	0.924	1.00	25.68
ATOM	2108	CB	SER	322	25.780	-0.082	2.322	1.00	27.15
ATOM	2109	OG	SER	322	24.576	-0.068	3.078	1.00	23.17
ATOM	2110	C	SER	322	24.345	-0.170	0.303	1.00	22.83
ATOM	2111	O	SER	322	23.264	0.419	0.193	1.00	23.80
ATOM	2112	N	GLU	323	24.505	-1.440	-0.043	1.00	18.89
ATOM	2113	CA	GLU	323	23.406	-2.181	-0.628	1.00	18.36
ATOM	2114	CB	GLU	323	23.899	-3.470	-1.270	1.00	15.88
ATOM	2115	CG	GLU	323	23.139	-3.804	-2.525	1.00	16.76
ATOM	2116	CD	GLU	323	23.509	-2.900	-3.674	1.00	13.21
ATOM	2117	OE1	GLU	323	24.719	-2.705	-3.918	1.00	8.62
ATOM	2118	OE2	GLU	323	22.591	-2.378	-4.332	1.00	16.00
ATOM	2119	C	GLU	323	22.400	-2.498	0.465	1.00	16.65
ATOM	2120	O	GLU	323	21.194	-2.595	0.205	1.00	14.62
ATOM	2121	N	HIS	324	22.913	-2.648	1.690	1.00	19.20
ATOM	2122	CA	HIS	324	22.096	-2.938	2.868	1.00	12.46

FIG. 1KK

ATOM	2123	CB	HIS	324	22.981	-3.132	4.105	1.00	18.88
ATOM	2124	CG	HIS	324	22.200	-3.360	5.366	1.00	19.65
ATOM	2125	CD2	HIS	324	21.581	-4.464	5.845	1.00	15.42
ATOM	2126	ND1	HIS	324	21.924	-2.347	6.261	1.00	19.17
ATOM	2127	CE1	HIS	324	21.160	-2.815	7.230	1.00	20.86
ATOM	2128	NE2	HIS	324	20.937	-4.097	7.003	1.00	17.26
ATOM	2129	C	HIS	324	21.151	-1.782	3.115	1.00	11.45
ATOM	2130	O	HIS	324	19.954	-1.980	3.338	1.00	12.09
ATOM	2131	N	ASN	325	21.689	-0.568	3.065	1.00	12.08
ATOM	2132	CA	ASN	325	20.875	0.626	3.278	1.00	15.82
ATOM	2133	CB	ASN	325	21.758	1.876	3.403	1.00	18.70
ATOM	2134	CG	ASN	325	22.479	1.960	4.746	1.00	14.57
ATOM	2135	OD1	ASN	325	21.934	1.558	5.777	1.00	20.65
ATOM	2136	ND2	ASN	325	23.702	2.489	4.742	1.00	8.45
ATOM	2137	C	ASN	325	19.820	0.802	2.186	1.00	17.97
ATOM	2138	O	ASN	325	18.671	1.166	2.474	1.00	18.10
ATOM	2139	N	LYS	326	20.197	0.498	0.943	1.00	17.49
ATOM	2140	CA	LYS	326	19.279	0.599	-0.189	1.00	13.39
ATOM	2141	CB	LYS	326	20.015	0.328	-1.496	1.00	13.97
ATOM	2142	CG	LYS	326	20.891	1.471	-1.948	1.00	13.26
ATOM	2143	CD	LYS	326	21.753	1.047	-3.118	1.00	16.38
ATOM	2144	CE	LYS	326	22.596	2.202	-3.628	1.00	18.48
ATOM	2145	NZ	LYS	326	23.721	1.752	-4.511	1.00	20.03
ATOM	2146	C	LYS	326	18.111	-0.367	-0.043	1.00	12.95
ATOM	2147	O	LYS	326	16.955	0.008	-0.263	1.00	17.37
ATOM	2148	N	LEU	327	18.402	-1.599	0.365	1.00	8.13
ATOM	2149	CA	LEU	327	17.362	-2.605	0.549	1.00	6.10
ATOM	2150	CB	LEU	327	17.992	-3.973	0.798	1.00	10.78
ATOM	2151	CG	LEU	327	17.045	-5.113	1.171	1.00	5.81
ATOM	2152	CD1	LEU	327	16.166	-5.466	-0.012	1.00	8.81
ATOM	2153	CD2	LEU	327	17.852	-6.305	1.610	1.00	2.24
ATOM	2154	C	LEU	327	16.438	-2.251	1.708	1.00	7.31
ATOM	2155	O	LEU	327	15.217	-2.409	1.609	1.00	9.49
ATOM	2156	N	LYS	328	17.026	-1.785	2.809	1.00	5.63
ATOM	2157	CA	LYS	328	16.252	-1.402	3.985	1.00	5.88
ATOM	2158	CB	LYS	328	17.166	-1.179	5.191	1.00	10.06
ATOM	2159	CG	LYS	328	17.780	-2.465	5.720	1.00	11.60
ATOM	2160	CD	LYS	328	16.679	-3.468	6.024	1.00	8.26
ATOM	2161	CE	LYS	328	17.231	-4.789	6.516	1.00	7.01
ATOM	2162	NZ	LYS	328	16.118	-5.682	6.946	1.00	9.67
ATOM	2163	C	LYS	328	15.422	-0.165	3.725	1.00	5.26
ATOM	2164	O	LYS	328	14.284	-0.064	4.193	1.00	5.47
ATOM	2165	N	ALA	329	15.981	0.763	2.954	1.00	4.26
ATOM	2166	CA	ALA	329	15.291	1.997	2.624	1.00	5.46
ATOM	2167	CB	ALA	329	16.196	2.911	1.825	1.00	8.76
ATOM	2168	C	ALA	329	14.024	1.676	1.845	1.00	8.00
ATOM	2169	O	ALA	329	12.987	2.308	2.054	1.00	12.88
ATOM	2170	N	SER	330	14.095	0.665	0.975	1.00	12.20
ATOM	2171	CA	SER	330	12.933	0.244	0.184	1.00	12.36
ATOM	2172	CB	SER	330	13.363	-0.524	-1.070	1.00	14.81
ATOM	2173	OG	SER	330	14.281	-1.556	-0.770	1.00	19.19
ATOM	2174	C	SER	330	11.929	-0.560	1.019	1.00	9.23
ATOM	2175	O	SER	330	10.715	-0.437	0.841	1.00	9.24
ATOM	2176	N	GLN	331	12.439	-1.344	1.966	1.00	14.64
ATOM	2177	CA	GLN	331	11.580	-2.128	2.861	1.00	13.55
ATOM	2178	CB	GLN	331	12.409	-3.181	3.608	1.00	14.40
ATOM	2179	CG	GLN	331	12.776	-4.408	2.764	1.00	16.36
ATOM	2180	CD	GLN	331	13.811	-5.308	3.417	1.00	15.16
ATOM	2181	OE1	GLN	331	14.614	-4.868	4.232	1.00	17.13

FIG. 1LL

ATOM	2182	NE2	GLN	331	13.811	-6.577	3.037	1.00	24.53
ATOM	2183	C	GLN	331	10.835	-1.211	3.851	1.00	10.18
ATOM	2184	O	GLN	331	9.673	-1.460	4.199	1.00	11.53
ATOM	2185	N	ALA	332	11.490	-0.135	4.275	1.00	6.48
ATOM	2186	CA	ALA	332	10.876	0.809	5.194	1.00	4.04
ATOM	2187	CB	ALA	332	11.871	1.849	5.605	1.00	2.00
ATOM	2188	C	ALA	332	9.734	1.456	4.451	1.00	10.26
ATOM	2189	O	ALA	332	8.584	1.433	4.900	1.00	10.60
ATOM	2190	N	ARG	333	10.055	1.927	3.246	1.00	15.77
ATOM	2191	CA	ARG	333	9.110	2.584	2.351	1.00	13.48
ATOM	2192	CB	ARG	333	9.848	3.065	1.104	1.00	14.31
ATOM	2193	CG	ARG	333	9.063	3.999	0.204	1.00	12.38
ATOM	2194	CD	ARG	333	9.895	4.319	-1.017	1.00	11.06
ATOM	2195	NE	ARG	333	11.106	5.055	-0.679	1.00	10.28
ATOM	2196	CZ	ARG	333	12.307	4.814	-1.194	1.00	17.30
ATOM	2197	NH1	ARG	333	12.477	3.847	-2.082	1.00	23.65
ATOM	2198	NH2	ARG	333	13.350	5.539	-0.809	1.00	18.12
ATOM	2199	C	ARG	333	7.979	1.620	1.984	1.00	13.96
ATOM	2200	O	ARG	333	6.823	2.038	1.867	1.00	15.40
ATOM	2201	N	ASP	334	8.300	0.328	1.854	1.00	10.58
ATOM	2202	CA	ASP	334	7.302	-0.696	1.538	1.00	11.35
ATOM	2203	CB	ASP	334	7.970	-2.037	1.211	1.00	20.54
ATOM	2204	CG	ASP	334	6.956	-3.141	0.915	1.00	24.07
ATOM	2205	OD1	ASP	334	6.077	-2.941	0.046	1.00	30.63
ATOM	2206	OD2	ASP	334	7.037	-4.213	1.553	1.00	26.21
ATOM	2207	C	ASP	334	6.358	-0.877	2.722	1.00	9.90
ATOM	2208	O	ASP	334	5.140	-0.961	2.560	1.00	10.84
ATOM	2209	N	LEU	335	6.922	-0.950	3.920	1.00	9.79
ATOM	2210	CA	LEU	335	6.111	-1.095	5.116	1.00	8.58
ATOM	2211	CB	LEU	335	7.019	-1.148	6.335	1.00	11.28
ATOM	2212	CG	LEU	335	6.454	-1.421	7.728	1.00	7.73
ATOM	2213	CD1	LEU	335	5.444	-2.553	7.731	1.00	4.16
ATOM	2214	CD2	LEU	335	7.624	-1.740	8.626	1.00	6.63
ATOM	2215	C	LEU	335	5.173	0.099	5.197	1.00	6.79
ATOM	2216	O	LEU	335	3.965	-0.062	5.362	1.00	8.39
ATOM	2217	N	LEU	336	5.738	1.287	4.993	1.00	4.95
ATOM	2218	CA	LEU	336	4.996	2.548	5.016	1.00	5.17
ATOM	2219	CB	LEU	336	5.933	3.713	4.691	1.00	2.00
ATOM	2220	CG	LEU	336	6.763	4.238	5.867	1.00	3.17
ATOM	2221	CD1	LEU	336	8.067	4.872	5.418	1.00	2.00
ATOM	2222	CD2	LEU	336	5.907	5.210	6.658	1.00	2.00
ATOM	2223	C	LEU	336	3.829	2.527	4.044	1.00	7.82
ATOM	2224	O	LEU	336	2.728	2.963	4.380	1.00	7.70
ATOM	2225	N	SER	337	4.061	1.964	2.861	1.00	12.67
ATOM	2226	CA	SER	337	3.035	1.849	1.831	1.00	16.08
ATOM	2227	CB	SER	337	3.653	1.360	0.524	1.00	17.25
ATOM	2228	OG	SER	337	3.994	-0.012	0.602	1.00	16.83
ATOM	2229	C	SER	337	1.909	0.894	2.245	1.00	17.26
ATOM	2230	O	SER	337	0.786	1.000	1.743	1.00	19.04
ATOM	2231	N	LYS	338	2.227	-0.056	3.128	1.00	17.99
ATOM	2232	CA	LYS	338	1.256	-1.033	3.617	1.00	10.96
ATOM	2233	CB	LYS	338	1.965	-2.289	4.091	1.00	12.91
ATOM	2234	CG	LYS	338	2.830	-2.975	3.070	1.00	11.53
ATOM	2235	CD	LYS	338	2.082	-4.071	2.357	1.00	11.57
ATOM	2236	CE	LYS	338	3.033	-5.208	2.000	1.00	17.59
ATOM	2237	NZ	LYS	338	4.347	-4.736	1.464	1.00	5.95
ATOM	2238	C	LYS	338	0.460	-0.479	4.777	1.00	6.87
ATOM	2239	O	LYS	338	-0.737	-0.723	4.885	1.00	7.32
ATOM	2240	N	MET	339	1.128	0.262	5.655	1.00	10.96

FIG. 1MM

ATOM	2241	CA	MET	339	0.476	0.842	6.833	1.00	12.64
ATOM	2242	CB	MET	339	1.505	1.161	7.921	1.00	13.33
ATOM	2243	CG	MET	339	2.181	-0.061	8.514	1.00	13.21
ATOM	2244	SD	MET	339	3.475	0.357	9.675	1.00	17.84
ATOM	2245	CE	MET	339	3.218	-0.864	10.884	1.00	20.59
ATOM	2246	C	MET	339	-0.347	2.082	6.530	1.00	10.81
ATOM	2247	O	MET	339	-1.512	2.168	6.930	1.00	11.79
ATOM	2248	N	LEU	340	0.257	3.029	5.813	1.00	10.89
ATOM	2249	CA	LEU	340	-0.415	4.271	5.454	1.00	9.27
ATOM	2250	CB	LEU	340	0.598	5.366	5.118	1.00	7.51
ATOM	2251	CG	LEU	340	1.311	5.939	6.344	1.00	7.71
ATOM	2252	CD1	LEU	340	2.511	6.771	5.938	1.00	7.14
ATOM	2253	CD2	LEU	340	0.336	6.747	7.179	1.00	6.71
ATOM	2254	C	LEU	340	-1.390	4.082	4.310	1.00	10.12
ATOM	2255	O	LEU	340	-1.132	4.510	3.187	1.00	13.32
ATOM	2256	N	VAL	341	-2.528	3.465	4.624	1.00	5.63
ATOM	2257	CA	VAL	341	-3.581	3.205	3.656	1.00	4.39
ATOM	2258	CB	VAL	341	-3.689	1.693	3.360	1.00	7.19
ATOM	2259	CG1	VAL	341	-4.868	1.408	2.461	1.00	8.69
ATOM	2260	CG2	VAL	341	-2.399	1.195	2.714	1.00	8.14
ATOM	2261	C	VAL	341	-4.891	3.718	4.227	1.00	5.17
ATOM	2262	O	VAL	341	-5.314	3.288	5.290	1.00	15.43
ATOM	2263	N	ILE	342	-5.557	4.599	3.491	1.00	6.54
ATOM	2264	CA	ILE	342	-6.812	5.218	3.922	1.00	8.56
ATOM	2265	CB	ILE	342	-7.260	6.324	2.923	1.00	7.43
ATOM	2266	CG2	ILE	342	-8.616	6.906	3.297	1.00	2.37
ATOM	2267	CG1	ILE	342	-6.209	7.432	2.881	1.00	10.85
ATOM	2268	CD1	ILE	342	-6.577	8.551	1.933	1.00	13.32
ATOM	2269	C	ILE	342	-7.947	4.244	4.159	1.00	12.09
ATOM	2270	O	ILE	342	-8.858	4.534	4.930	1.00	18.08
ATOM	2271	N	ASP	343	-7.910	3.097	3.500	1.00	19.41
ATOM	2272	CA	ASP	343	-8.972	2.117	3.688	1.00	20.62
ATOM	2273	CB	ASP	343	-9.398	1.538	2.336	1.00	23.24
ATOM	2274	CG	ASP	343	-10.671	0.714	2.422	1.00	24.40
ATOM	2275	OD1	ASP	343	-11.556	1.024	3.248	1.00	28.91
ATOM	2276	OD2	ASP	343	-10.805	-0.243	1.638	1.00	33.68
ATOM	2277	C	ASP	343	-8.516	1.006	4.630	1.00	20.89
ATOM	2278	O	ASP	343	-7.448	0.417	4.446	1.00	24.41
ATOM	2279	N	PRO	344	-9.295	0.747	5.686	1.00	18.88
ATOM	2280	CD	PRO	344	-10.522	1.442	6.107	1.00	18.84
ATOM	2281	CA	PRO	344	-8.952	-0.306	6.641	1.00	17.35
ATOM	2282	CB	PRO	344	-10.148	-0.290	7.595	1.00	16.82
ATOM	2283	CG	PRO	344	-10.594	1.118	7.571	1.00	9.78
ATOM	2284	C	PRO	344	-8.865	-1.640	5.917	1.00	19.67
ATOM	2285	O	PRO	344	-7.942	-2.422	6.152	1.00	20.89
ATOM	2286	N	ALA	345	-9.811	-1.851	4.992	1.00	20.12
ATOM	2287	CA	ALA	345	-9.916	-3.077	4.192	1.00	15.83
ATOM	2288	CB	ALA	345	-11.200	-3.071	3.363	1.00	9.24
ATOM	2289	C	ALA	345	-8.726	-3.394	3.301	1.00	12.79
ATOM	2290	O	ALA	345	-8.619	-4.503	2.781	1.00	19.39
ATOM	2291	N	LYS	346	-7.853	-2.416	3.098	1.00	11.07
ATOM	2292	CA	LYS	346	-6.661	-2.617	2.288	1.00	11.20
ATOM	2293	CB	LYS	346	-6.628	-1.627	1.122	1.00	19.22
ATOM	2294	CG	LYS	346	-7.759	-1.824	0.123	1.00	21.98
ATOM	2295	CD	LYS	346	-7.699	-0.761	-0.950	1.00	31.16
ATOM	2296	CE	LYS	346	-8.808	-0.943	-1.970	1.00	35.66
ATOM	2297	NZ	LYS	346	-8.612	-2.174	-2.792	1.00	46.86
ATOM	2298	C	LYS	346	-5.428	-2.449	3.159	1.00	12.65
ATOM	2299	O	LYS	346	-4.313	-2.723	2.722	1.00	14.60

FIG. 1NN

ATOM	2300	N	ARG	347	-5.637	-2.018	4.403	1.00	18.46
ATOM	2301	CA	ARG	347	-4.544	-1.820	5.352	1.00	15.01
ATOM	2302	CB	ARG	347	-4.935	-0.811	6.433	1.00	13.75
ATOM	2303	CG	ARG	347	-3.733	-0.158	7.128	1.00	9.99
ATOM	2304	CD	ARG	347	-4.175	0.743	8.272	1.00	8.39
ATOM	2305	NE	ARG	347	-5.122	1.755	7.812	1.00	11.90
ATOM	2306	CZ	ARG	347	-6.130	2.242	8.529	1.00	14.87
ATOM	2307	NH1	ARG	347	-6.350	1.821	9.765	1.00	20.10
ATOM	2308	NH2	ARG	347	-6.945	3.137	7.995	1.00	13.60
ATOM	2309	C	ARG	347	-4.074	-3.133	6.003	1.00	15.98
ATOM	2310	O	ARG	347	-4.868	-4.024	6.321	1.00	18.25
ATOM	2311	N	ILE	348	-2.764	-3.221	6.204	1.00	12.17
ATOM	2312	CA	ILE	348	-2.088	-4.367	6.802	1.00	10.44
ATOM	2313	CB	ILE	348	-0.556	-4.152	6.681	1.00	2.00
ATOM	2314	CG2	ILE	348	-0.095	-3.082	7.655	1.00	4.05
ATOM	2315	CG1	ILE	348	0.198	-5.444	6.951	1.00	2.00
ATOM	2316	CD1	ILE	348	1.708	-5.293	6.822	1.00	3.75
ATOM	2317	C	ILE	348	-2.444	-4.519	8.286	1.00	15.07
ATOM	2318	O	ILE	348	-2.906	-3.565	8.912	1.00	24.64
ATOM	2319	N	SER	349	-2.222	-5.708	8.848	1.00	17.85
ATOM	2320	CA	SER	349	-2.500	-5.961	10.265	1.00	12.24
ATOM	2321	CB	SER	349	-3.243	-7.288	10.435	1.00	18.76
ATOM	2322	OG	SER	349	-2.400	-8.380	10.114	1.00	24.15
ATOM	2323	C	SER	349	-1.202	-5.990	11.093	1.00	13.20
ATOM	2324	O	SER	349	-0.089	-5.901	10.548	1.00	8.49
ATOM	2325	N	VAL	350	-1.353	-6.169	12.407	1.00	11.30
ATOM	2326	CA	VAL	350	-0.226	-6.196	13.338	1.00	4.95
ATOM	2327	CB	VAL	350	-0.711	-6.298	14.829	1.00	11.43
ATOM	2328	CG1	VAL	350	0.454	-6.071	15.780	1.00	8.45
ATOM	2329	CG2	VAL	350	-1.822	-5.269	15.122	1.00	7.42
ATOM	2330	C	VAL	350	0.732	-7.336	13.037	1.00	2.00
ATOM	2331	O	VAL	350	1.951	-7.153	12.998	1.00	2.70
ATOM	2332	N	ASP	351	0.192	-8.513	12.763	1.00	8.23
ATOM	2333	CA	ASP	351	1.059	-9.648	12.484	1.00	10.61
ATOM	2334	CB	ASP	351	0.284	-10.952	12.555	1.00	18.49
ATOM	2335	CG	ASP	351	0.210	-11.491	13.964	1.00	18.11
ATOM	2336	OD1	ASP	351	1.277	-11.903	14.470	1.00	22.45
ATOM	2337	OD2	ASP	351	-0.899	-11.495	14.546	1.00	14.05
ATOM	2338	C	ASP	351	1.863	-9.567	11.212	1.00	9.41
ATOM	2339	O	ASP	351	3.064	-9.841	11.221	1.00	11.00
ATOM	2340	N	ASP	352	1.222	-9.189	10.114	1.00	10.25
ATOM	2341	CA	ASP	352	1.950	-9.069	8.857	1.00	12.98
ATOM	2342	CB	ASP	352	1.010	-8.664	7.725	1.00	10.96
ATOM	2343	CG	ASP	352	-0.227	-9.525	7.649	1.00	12.21
ATOM	2344	OD1	ASP	352	-0.131	-10.756	7.855	1.00	12.96
ATOM	2345	OD2	ASP	352	-1.303	-8.959	7.374	1.00	15.38
ATOM	2346	C	ASP	352	3.018	-7.994	9.045	1.00	15.26
ATOM	2347	O	ASP	352	4.150	-8.133	8.569	1.00	18.07
ATOM	2348	N	ALA	353	2.660	-6.958	9.805	1.00	14.96
ATOM	2349	CA	ALA	353	3.552	-5.846	10.092	1.00	10.83
ATOM	2350	CB	ALA	353	2.796	-4.737	10.805	1.00	14.35
ATOM	2351	C	ALA	353	4.734	-6.332	10.927	1.00	10.55
ATOM	2352	O	ALA	353	5.864	-5.892	10.716	1.00	10.08
ATOM	2353	N	LEU	354	4.481	-7.282	11.831	1.00	10.79
ATOM	2354	CA	LEU	354	5.529	-7.848	12.683	1.00	7.58
ATOM	2355	CB	LEU	354	4.917	-8.549	13.900	1.00	8.36
ATOM	2356	CG	LEU	354	4.569	-7.702	15.136	1.00	5.81
ATOM	2357	CD1	LEU	354	3.437	-8.329	15.905	1.00	3.35
ATOM	2358	CD2	LEU	354	5.789	-7.506	16.029	1.00	2.00

FIG. 100

ATOM	2359	C	LEU	354	6.400	-8.824	11.906	1.00	7.39
ATOM	2360	O	LEU	354	7.616	-8.906	12.116	1.00	2.00
ATOM	2361	N	GLN	355	5.763	-9.534	10.979	1.00	9.55
ATOM	2362	CA	GLN	355	6.438	-10.522	10.144	1.00	13.96
ATOM	2363	CB	GLN	355	5.440	-11.586	9.672	1.00	13.47
ATOM	2364	CG	GLN	355	4.848	-12.460	10.767	1.00	12.65
ATOM	2365	CD	GLN	355	5.647	-13.716	11.003	1.00	19.49
ATOM	2366	OE1	GLN	355	6.837	-13.668	11.318	1.00	21.81
ATOM	2367	NE2	GLN	355	4.997	-14.859	10.842	1.00	21.15
ATOM	2368	C	GLN	355	7.107	-9.893	8.925	1.00	15.16
ATOM	2369	O	GLN	355	7.853	-10.561	8.228	1.00	16.20
ATOM	2370	N	HIS	356	6.837	-8.614	8.675	1.00	15.76
ATOM	2371	CA	HIS	356	7.388	-7.889	7.530	1.00	9.95
ATOM	2372	CB	HIS	356	6.817	-6.469	7.534	1.00	7.19
ATOM	2373	CG	HIS	356	7.175	-5.666	6.320	1.00	5.18
ATOM	2374	CD2	HIS	356	6.426	-5.261	5.277	1.00	2.47
ATOM	2375	ND1	HIS	356	8.457	-5.216	6.076	1.00	3.37
ATOM	2376	CE1	HIS	356	8.481	-4.577	4.923	1.00	8.01
ATOM	2377	NE2	HIS	356	7.261	-4.587	4.416	1.00	9.88
ATOM	2378	C	HIS	356	8.922	-7.838	7.558	1.00	11.50
ATOM	2379	O	HIS	356	9.501	-7.569	8.597	1.00	15.45
ATOM	2380	N	PRO	357	9.593	-8.064	6.409	1.00	14.61
ATOM	2381	CD	PRO	357	8.977	-8.395	5.114	1.00	16.32
ATOM	2382	CA	PRO	357	11.065	-8.045	6.276	1.00	12.00
ATOM	2383	CB	PRO	357	11.287	-8.137	4.756	1.00	14.38
ATOM	2384	CG	PRO	357	9.955	-7.764	4.152	1.00	16.33
ATOM	2385	C	PRO	357	11.821	-6.863	6.889	1.00	13.41
ATOM	2386	O	PRO	357	13.036	-6.957	7.112	1.00	16.91
ATOM	2387	N	TYR	358	11.140	-5.739	7.113	1.00	15.19
ATOM	2388	CA	TYR	358	11.778	-4.570	7.737	1.00	16.88
ATOM	2389	CB	TYR	358	11.053	-3.251	7.379	1.00	11.17
ATOM	2390	CG	TYR	358	11.801	-2.025	7.881	1.00	7.46
ATOM	2391	CD1	TYR	358	13.148	-1.848	7.585	1.00	5.18
ATOM	2392	CE1	TYR	358	13.870	-0.783	8.112	1.00	8.86
ATOM	2393	CD2	TYR	358	11.193	-1.084	8.718	1.00	9.39
ATOM	2394	CE2	TYR	358	11.918	-0.010	9.252	1.00	2.00
ATOM	2395	CZ	TYR	358	13.255	0.126	8.944	1.00	4.61
ATOM	2396	OH	TYR	358	14.007	1.150	9.469	1.00	4.98
ATOM	2397	C	TYR	358	11.781	-4.733	9.271	1.00	17.22
ATOM	2398	O	TYR	358	12.697	-4.272	9.949	1.00	16.24
ATOM	2399	N	ILE	359	10.772	-5.432	9.789	1.00	16.60
ATOM	2400	CA	ILE	359	10.589	-5.650	11.217	1.00	14.11
ATOM	2401	CB	ILE	359	9.093	-5.480	11.579	1.00	16.20
ATOM	2402	CG2	ILE	359	8.878	-5.617	13.084	1.00	19.56
ATOM	2403	CG1	ILE	359	8.560	-4.143	11.074	1.00	5.87
ATOM	2404	CD1	ILE	359	9.255	-2.942	11.659	1.00	13.16
ATOM	2405	C	ILE	359	11.029	-6.996	11.798	1.00	15.39
ATOM	2406	O	ILE	359	11.676	-7.037	12.842	1.00	16.24
ATOM	2407	N	ASN	360	10.681	-8.091	11.128	1.00	14.64
ATOM	2408	CA	ASN	360	10.982	-9.445	11.604	1.00	9.97
ATOM	2409	CB	ASN	360	10.424	-10.494	10.644	1.00	7.20
ATOM	2410	CG	ASN	360	11.133	-10.506	9.304	1.00	3.95
ATOM	2411	OD1	ASN	360	12.359	-10.382	9.213	1.00	2.00
ATOM	2412	ND2	ASN	360	10.369	-10.721	8.259	1.00	2.26
ATOM	2413	C	ASN	360	12.401	-9.837	12.007	1.00	13.06
ATOM	2414	O	ASN	360	12.610	-10.963	12.441	1.00	18.34
ATOM	2415	N	VAL	361	13.381	-8.949	11.863	1.00	16.41
ATOM	2416	CA	VAL	361	14.743	-9.295	12.274	1.00	19.73
ATOM	2417	CB	VAL	361	15.812	-8.278	11.768	1.00	19.18

FIG. 1PP

ATOM	2418	CG1	VAL	361	15.998	-8.423	10.277	1.00	23.78
ATOM	2419	CG2	VAL	361	15.412	-6.860	12.104	1.00	11.95
ATOM	2420	C	VAL	361	14.829	-9.400	13.803	1.00	24.53
ATOM	2421	O	VAL	361	15.733	-10.048	14.341	1.00	28.66
ATOM	2422	N	TRP	362	13.886	-8.758	14.496	1.00	23.87
ATOM	2423	CA	TRP	362	13.835	-8.778	15.960	1.00	18.58
ATOM	2424	CB	TRP	362	13.483	-7.392	16.521	1.00	12.66
ATOM	2425	CG	TRP	362	14.272	-6.282	15.991	1.00	4.45
ATOM	2426	CD2	TRP	362	15.653	-6.011	16.254	1.00	4.23
ATOM	2427	CE2	TRP	362	15.987	-4.843	15.536	1.00	2.00
ATOM	2428	CE3	TRP	362	16.631	-6.646	17.017	1.00	2.00
ATOM	2429	CD1	TRP	362	13.836	-5.301	15.162	1.00	2.00
ATOM	2430	NE1	TRP	362	14.860	-4.431	14.881	1.00	2.00
ATOM	2431	CZ2	TRP	362	17.270	-4.289	15.568	1.00	2.00
ATOM	2432	CZ3	TRP	362	17.901	-6.100	17.051	1.00	7.07
ATOM	2433	CH2	TRP	362	18.212	-4.930	16.324	1.00	8.63
ATOM	2434	C	TRP	362	12.742	-9.730	16.425	1.00	20.11
ATOM	2435	O	TRP	362	12.514	-9.871	17.626	1.00	19.34
ATOM	2436	N	TYR	363	12.045	-10.363	15.488	1.00	15.68
ATOM	2437	CA	TYR	363	10.960	-11.246	15.851	1.00	12.75
ATOM	2438	CB	TYR	363	10.319	-11.853	14.611	1.00	4.47
ATOM	2439	CG	TYR	363	8.891	-12.294	14.820	1.00	7.70
ATOM	2440	CD1	TYR	363	8.582	-13.571	15.297	1.00	6.58
ATOM	2441	CE1	TYR	363	7.240	-13.975	15.468	1.00	2.00
ATOM	2442	CD2	TYR	363	7.837	-11.441	14.523	1.00	2.00
ATOM	2443	CE2	TYR	363	6.511	-11.836	14.688	1.00	5.09
ATOM	2444	CZ	TYR	363	6.218	-13.100	15.158	1.00	4.18
ATOM	2445	OH	TYR	363	4.898	-13.484	15.291	1.00	15.76
ATOM	2446	C	TYR	363	11.413	-12.336	16.812	1.00	16.54
ATOM	2447	O	TYR	363	12.380	-13.057	16.556	1.00	20.38
ATOM	2448	N	ASP	364	10.755	-12.380	17.962	1.00	15.31
ATOM	2449	CA	ASP	364	11.018	-13.366	18.999	1.00	10.29
ATOM	2450	CB	ASP	364	11.843	-12.765	20.134	1.00	12.82
ATOM	2451	CG	ASP	364	12.149	-13.764	21.222	1.00	13.30
ATOM	2452	OD1	ASP	364	11.196	-14.281	21.823	1.00	11.59
ATOM	2453	OD2	ASP	364	13.337	-14.040	21.472	1.00	14.16
ATOM	2454	C	ASP	364	9.613	-13.658	19.458	1.00	9.97
ATOM	2455	O	ASP	364	8.919	-12.772	19.943	1.00	14.45
ATOM	2456	N	PRO	365	9.168	-14.907	19.316	1.00	9.41
ATOM	2457	CD	PRO	365	9.886	-16.099	18.829	1.00	3.16
ATOM	2458	CA	PRO	365	7.802	-15.234	19.735	1.00	5.93
ATOM	2459	CB	PRO	365	7.636	-16.668	19.238	1.00	2.73
ATOM	2460	CG	PRO	365	9.031	-17.222	19.340	1.00	2.00
ATOM	2461	C	PRO	365	7.472	-15.053	21.217	1.00	5.07
ATOM	2462	O	PRO	365	6.299	-15.029	21.603	1.00	3.26
ATOM	2463	N	ALA	366	8.499	-14.888	22.040	1.00	5.56
ATOM	2464	CA	ALA	366	8.292	-14.690	23.472	1.00	13.27
ATOM	2465	CB	ALA	366	9.589	-14.902	24.231	1.00	16.70
ATOM	2466	C	ALA	366	7.758	-13.284	23.717	1.00	14.41
ATOM	2467	O	ALA	366	6.762	-13.107	24.422	1.00	19.61
ATOM	2468	N	GLU	367	8.385	-12.302	23.063	1.00	15.02
ATOM	2469	CA	GLU	367	8.009	-10.883	23.164	1.00	5.43
ATOM	2470	CB	GLU	367	9.123	-9.999	22.619	1.00	2.00
ATOM	2471	CG	GLU	367	10.456	-10.213	23.322	1.00	3.66
ATOM	2472	CD	GLU	367	11.566	-9.341	22.783	1.00	7.74
ATOM	2473	OE1	GLU	367	12.728	-9.525	23.205	1.00	2.97
ATOM	2474	OE2	GLU	367	11.286	-8.467	21.936	1.00	12.02
ATOM	2475	C	GLU	367	6.742	-10.599	22.398	1.00	5.07
ATOM	2476	O	GLU	367	5.875	-9.878	22.881	1.00	2.04

FIG. 1QQ

ATOM	2477	N	VAL	368	6.621	-11.197	21.215	1.00	7.87
ATOM	2478	CA	VAL	368	5.447	-10.995	20.378	1.00	7.65
ATOM	2479	CB	VAL	368	5.653	-11.535	18.924	1.00	12.19
ATOM	2480	CG1	VAL	368	4.330	-11.532	18.156	1.00	9.04
ATOM	2481	CG2	VAL	368	6.691	-10.684	18.169	1.00	2.75
ATOM	2482	C	VAL	368	4.234	-11.656	20.998	1.00	7.96
ATOM	2483	O	VAL	368	3.175	-11.042	21.109	1.00	15.88
ATOM	2484	N	ALA	369	4.395	-12.901	21.428	1.00	17.86
ATOM	2485	CA	ALA	369	3.295	-13.640	22.039	1.00	25.19
ATOM	2486	CB	ALA	369	3.167	-15.013	21.382	1.00	23.81
ATOM	2487	C	ALA	369	3.389	-13.774	23.572	1.00	30.10
ATOM	2488	O	ALA	369	3.801	-14.814	24.096	1.00	36.36
ATOM	2489	N	ALA	370	3.029	-12.706	24.275	1.00	27.76
ATOM	2490	CA	ALA	370	3.030	-12.678	25.731	1.00	23.19
ATOM	2491	CB	ALA	370	3.916	-11.564	26.236	1.00	19.06
ATOM	2492	C	ALA	370	1.578	-12.411	26.105	1.00	25.30
ATOM	2493	O	ALA	370	1.068	-11.327	25.856	1.00	28.84
ATOM	2494	N	PRO	371	0.895	-13.398	26.695	1.00	30.05
ATOM	2495	CD	PRO	371	1.442	-14.670	27.208	1.00	30.56
ATOM	2496	CA	PRO	371	-0.520	-13.238	27.085	1.00	30.50
ATOM	2497	CB	PRO	371	-0.867	-14.618	27.647	1.00	29.26
ATOM	2498	CG	PRO	371	0.434	-15.060	28.275	1.00	31.17
ATOM	2499	C	PRO	371	-0.740	-12.117	28.109	1.00	29.61
ATOM	2500	O	PRO	371	0.153	-11.801	28.895	1.00	28.65
ATOM	2501	N	PRO	372	-1.924	-11.473	28.065	1.00	29.10
ATOM	2502	CD	PRO	372	-2.933	-11.710	27.024	1.00	31.05
ATOM	2503	CA	PRO	372	-2.347	-10.381	28.954	1.00	32.89
ATOM	2504	CB	PRO	372	-3.551	-9.797	28.208	1.00	26.47
ATOM	2505	CG	PRO	372	-4.159	-11.002	27.577	1.00	27.14
ATOM	2506	C	PRO	372	-2.733	-10.848	30.363	1.00	37.35
ATOM	2507	O	PRO	372	-3.280	-11.974	30.476	1.00	41.20
ATOM	2508	CB	ALA	382	-17.334	3.104	28.970	1.00	45.07
ATOM	2509	C	ALA	382	-19.469	3.190	30.278	1.00	43.41
ATOM	2510	O	ALA	382	-20.418	2.982	29.516	1.00	43.69
ATOM	2511	N	ALA	382	-18.413	1.010	29.750	1.00	45.59
ATOM	2512	CA	ALA	382	-18.152	2.445	30.082	1.00	44.95
ATOM	2513	N	ALA	383	-19.519	4.055	31.291	1.00	40.49
ATOM	2514	CA	ALA	383	-20.721	4.832	31.581	1.00	37.23
ATOM	2515	CB	ALA	383	-21.499	4.204	32.734	1.00	35.88
ATOM	2516	C	ALA	383	-20.408	6.290	31.888	1.00	35.44
ATOM	2517	O	ALA	383	-19.252	6.663	32.105	1.00	33.54
ATOM	2518	N	GLU	384	-21.450	7.112	31.885	1.00	33.22
ATOM	2519	CA	GLU	384	-21.306	8.531	32.161	1.00	35.14
ATOM	2520	CB	GLU	384	-22.190	9.354	31.209	1.00	39.93
ATOM	2521	CG	GLU	384	-21.976	9.069	29.712	1.00	44.06
ATOM	2522	CD	GLU	384	-20.563	9.377	29.214	1.00	47.10
ATOM	2523	OE1	GLU	384	-19.986	10.411	29.611	1.00	47.81
ATOM	2524	OE2	GLU	384	-20.029	8.581	28.413	1.00	50.85
ATOM	2525	C	GLU	384	-21.689	8.804	33.614	1.00	34.52
ATOM	2526	O	GLU	384	-22.774	8.430	34.065	1.00	33.70
ATOM	2527	N	HIS	385	-20.783	9.442	34.348	1.00	31.42
ATOM	2528	CA	HIS	385	-21.029	9.759	35.751	1.00	27.96
ATOM	2529	CB	HIS	385	-20.070	8.981	36.652	1.00	26.39
ATOM	2530	CG	HIS	385	-20.098	7.501	36.448	1.00	24.59
ATOM	2531	CD2	HIS	385	-19.113	6.626	36.149	1.00	27.17
ATOM	2532	ND1	HIS	385	-21.260	6.762	36.532	1.00	27.18
ATOM	2533	CE1	HIS	385	-20.984	5.492	36.292	1.00	26.97
ATOM	2534	NE2	HIS	385	-19.691	5.380	36.057	1.00	27.51
ATOM	2535	C	HIS	385	-20.862	11.247	36.009	1.00	29.29

FIG. 1RR

ATOM	2536	O	HIS	385	-20.400	11.993	35.143	1.00	31.45
ATOM	2537	N	THR	386	-21.234	11.673	37.211	1.00	24.31
ATOM	2538	CA	THR	386	-21.111	13.067	37.594	1.00	17.05
ATOM	2539	CB	THR	386	-22.149	13.439	38.661	1.00	18.48
ATOM	2540	OG1	THR	386	-21.927	12.653	39.835	1.00	26.84
ATOM	2541	CG2	THR	386	-23.557	13.185	38.152	1.00	14.58
ATOM	2542	C	THR	386	-19.713	13.286	38.147	1.00	18.26
ATOM	2543	O	THR	386	-18.908	12.358	38.198	1.00	16.54
ATOM	2544	N	ILE	387	-19.425	14.514	38.560	1.00	22.20
ATOM	2545	CA	ILE	387	-18.127	14.854	39.120	1.00	24.81
ATOM	2546	CB	ILE	387	-18.003	16.371	39.363	1.00	26.15
ATOM	2547	CG2	ILE	387	-16.738	16.690	40.164	1.00	20.29
ATOM	2548	CG1	ILE	387	-18.015	17.107	38.023	1.00	26.13
ATOM	2549	CD1	ILE	387	-18.028	18.611	38.164	1.00	30.51
ATOM	2550	C	ILE	387	-17.978	14.144	40.446	1.00	29.13
ATOM	2551	O	ILE	387	-16.919	13.591	40.744	1.00	36.90
ATOM	2552	N	ALA	388	-19.049	14.151	41.235	1.00	28.74
ATOM	2553	CA	ALA	388	-19.028	13.504	42.539	1.00	27.98
ATOM	2554	CB	ALA	388	-20.269	13.869	43.331	1.00	24.16
ATOM	2555	C	ALA	388	-18.913	12.000	42.356	1.00	27.08
ATOM	2556	O	ALA	388	-18.120	11.351	43.035	1.00	28.54
ATOM	2557	N	GLU	389	-19.647	11.461	41.385	1.00	27.57
ATOM	2558	CA	GLU	389	-19.611	10.025	41.102	1.00	25.55
ATOM	2559	CB	GLU	389	-20.753	9.637	40.169	1.00	20.07
ATOM	2560	CG	GLU	389	-22.115	9.902	40.776	1.00	17.01
ATOM	2561	CD	GLU	389	-23.257	9.727	39.794	1.00	22.78
ATOM	2562	OE1	GLU	389	-23.013	9.643	38.572	1.00	24.62
ATOM	2563	OE2	GLU	389	-24.417	9.690	40.245	1.00	26.31
ATOM	2564	C	GLU	389	-18.265	9.572	40.530	1.00	27.33
ATOM	2565	O	GLU	389	-17.818	8.461	40.819	1.00	35.55
ATOM	2566	N	TRP	390	-17.611	10.438	39.756	1.00	24.95
ATOM	2567	CA	TRP	390	-16.309	10.124	39.179	1.00	22.08
ATOM	2568	CB	TRP	390	-15.975	11.055	37.995	1.00	26.49
ATOM	2569	CG	TRP	390	-16.480	10.612	36.619	1.00	31.67
ATOM	2570	CD2	TRP	390	-16.260	9.335	35.968	1.00	29.90
ATOM	2571	CE2	TRP	390	-16.914	9.391	34.714	1.00	28.93
ATOM	2572	CE3	TRP	390	-15.580	8.164	36.323	1.00	27.49
ATOM	2573	CD1	TRP	390	-17.229	11.356	35.747	1.00	31.50
ATOM	2574	NE1	TRP	390	-17.493	10.630	34.606	1.00	32.29
ATOM	2575	CZ2	TRP	390	-16.903	8.316	33.819	1.00	29.75
ATOM	2576	CZ3	TRP	390	-15.569	7.102	35.437	1.00	29.76
ATOM	2577	CH2	TRP	390	-16.229	7.183	34.198	1.00	31.94
ATOM	2578	C	TRP	390	-15.207	10.266	40.227	1.00	21.39
ATOM	2579	O	TRP	390	-14.144	9.661	40.100	1.00	26.37
ATOM	2580	N	LYS	391	-15.453	11.085	41.245	1.00	19.83
ATOM	2581	CA	LYS	391	-14.484	11.323	42.314	1.00	16.84
ATOM	2582	CB	LYS	391	-14.925	12.544	43.132	1.00	14.49
ATOM	2583	CG	LYS	391	-13.951	13.006	44.213	1.00	10.70
ATOM	2584	CD	LYS	391	-14.510	14.218	44.963	1.00	13.44
ATOM	2585	CE	LYS	391	-13.478	14.846	45.906	1.00	8.99
ATOM	2586	NZ	LYS	391	-14.038	16.018	46.657	1.00	9.86
ATOM	2587	C	LYS	391	-14.328	10.102	43.231	1.00	18.26
ATOM	2588	O	LYS	391	-13.214	9.769	43.654	1.00	15.87
ATOM	2589	N	GLU	392	-15.451	9.443	43.522	1.00	20.49
ATOM	2590	CA	GLU	392	-15.483	8.267	44.386	1.00	23.22
ATOM	2591	CB	GLU	392	-16.924	7.953	44.777	1.00	26.59
ATOM	2592	CG	GLU	392	-17.050	6.956	45.911	1.00	36.07
ATOM	2593	CD	GLU	392	-18.359	7.099	46.663	1.00	41.89
ATOM	2594	OE1	GLU	392	-18.310	7.239	47.902	1.00	41.27

FIG. 1SS

ATOM	2595	OE2	GLU	392	-19.432	7.071	46.018	1.00	50.99
ATOM	2596	C	GLU	392	-14.840	7.052	43.737	1.00	22.68
ATOM	2597	O	GLU	392	-14.103	6.304	44.389	1.00	23.88
ATOM	2598	N	LEU	393	-15.137	6.853	42.455	1.00	20.40
ATOM	2599	CA	LEU	393	-14.583	5.746	41.693	1.00	14.24
ATOM	2600	CB	LEU	393	-15.141	5.763	40.280	1.00	9.57
ATOM	2601	CG	LEU	393	-16.578	5.266	40.243	1.00	13.19
ATOM	2602	CD1	LEU	393	-17.203	5.553	38.884	1.00	5.67
ATOM	2603	CD2	LEU	393	-16.579	3.772	40.580	1.00	12.28
ATOM	2604	C	LEU	393	-13.067	5.846	41.648	1.00	15.60
ATOM	2605	O	LEU	393	-12.369	4.894	41.995	1.00	21.88
ATOM	2606	N	ILE	394	-12.566	7.022	41.278	1.00	15.30
ATOM	2607	CA	ILE	394	-11.133	7.280	41.183	1.00	13.08
ATOM	2608	CB	ILE	394	-10.856	8.709	40.595	1.00	12.22
ATOM	2609	CG2	ILE	394	-9.353	9.003	40.512	1.00	6.65
ATOM	2610	CG1	ILE	394	-11.476	8.825	39.199	1.00	10.42
ATOM	2611	CD1	ILE	394	-11.308	10.181	38.555	1.00	13.03
ATOM	2612	C	ILE	394	-10.465	7.145	42.545	1.00	10.70
ATOM	2613	O	ILE	394	-9.296	6.751	42.624	1.00	8.46
ATOM	2614	N	TYR	395	-11.198	7.470	43.612	1.00	13.66
ATOM	2615	CA	TYR	395	-10.652	7.377	44.966	1.00	13.63
ATOM	2616	CB	TYR	395	-11.518	8.160	45.957	1.00	15.60
ATOM	2617	CG	TYR	395	-10.902	8.313	47.328	1.00	16.11
ATOM	2618	CD1	TYR	395	-9.631	8.867	47.496	1.00	10.10
ATOM	2619	CE1	TYR	395	-9.063	8.992	48.756	1.00	17.16
ATOM	2620	CD2	TYR	395	-11.585	7.891	48.463	1.00	21.34
ATOM	2621	CE2	TYR	395	-11.024	8.012	49.729	1.00	21.42
ATOM	2622	CZ	TYR	395	-9.767	8.559	49.871	1.00	22.71
ATOM	2623	OH	TYR	395	-9.233	8.648	51.133	1.00	19.28
ATOM	2624	C	TYR	395	-10.560	5.915	45.366	1.00	13.33
ATOM	2625	O	TYR	395	-9.488	5.432	45.741	1.00	11.26
ATOM	2626	N	LYS	396	-11.667	5.196	45.209	1.00	12.67
ATOM	2627	CA	LYS	396	-11.718	3.783	45.536	1.00	20.01
ATOM	2628	CB	LYS	396	-13.112	3.220	45.276	1.00	26.69
ATOM	2629	CG	LYS	396	-14.136	3.554	46.350	1.00	25.29
ATOM	2630	CD	LYS	396	-15.474	2.913	46.019	1.00	28.95
ATOM	2631	CE	LYS	396	-16.543	3.291	47.026	1.00	28.60
ATOM	2632	NZ	LYS	396	-17.906	2.976	46.513	1.00	33.35
ATOM	2633	C	LYS	396	-10.690	2.989	44.747	1.00	22.43
ATOM	2634	O	LYS	396	-10.143	2.010	45.250	1.00	26.83
ATOM	2635	N	GLU	397	-10.402	3.420	43.525	1.00	19.52
ATOM	2636	CA	GLU	397	-9.427	2.720	42.711	1.00	18.90
ATOM	2637	CB	GLU	397	-9.590	3.106	41.241	1.00	19.12
ATOM	2638	CG	GLU	397	-9.221	2.003	40.254	1.00	18.47
ATOM	2639	CD	GLU	397	-10.160	0.826	40.325	1.00	18.19
ATOM	2640	OE1	GLU	397	-9.669	-0.323	40.333	1.00	27.13
ATOM	2641	OE2	GLU	397	-11.390	1.044	40.384	1.00	14.60
ATOM	2642	C	GLU	397	-8.004	3.014	43.197	1.00	20.33
ATOM	2643	O	GLU	397	-7.128	2.156	43.119	1.00	22.46
ATOM	2644	N	VAL	398	-7.792	4.211	43.741	1.00	25.23
ATOM	2645	CA	VAL	398	-6.478	4.635	44.242	1.00	23.12
ATOM	2646	CB	VAL	398	-6.339	6.197	44.207	1.00	22.95
ATOM	2647	CG1	VAL	398	-4.986	6.648	44.761	1.00	22.77
ATOM	2648	CG2	VAL	398	-6.520	6.706	42.774	1.00	22.38
ATOM	2649	C	VAL	398	-6.175	4.128	45.660	1.00	26.11
ATOM	2650	O	VAL	398	-5.001	3.982	46.053	1.00	22.73
ATOM	2651	N	MET	399	-7.230	3.822	46.413	1.00	27.64
ATOM	2652	CA	MET	399	-7.075	3.339	47.781	1.00	33.11
ATOM	2653	CB	MET	399	-8.149	3.953	48.680	1.00	34.03

FIG. 1TT

ATOM	2654	CG	MET	399	-7.994	5.465	48.863	1.00	29.75
ATOM	2655	SD	MET	399	-6.663	5.989	50.009	1.00	40.78
ATOM	2656	CE	MET	399	-5.137	5.902	49.010	1.00	35.81
ATOM	2657	C	MET	399	-7.015	1.820	47.942	1.00	36.50
ATOM	2658	O	MET	399	-6.886	1.323	49.063	1.00	38.05
ATOM	2659	N	ASN	400	-7.108	1.092	46.829	1.00	41.19
ATOM	2660	CA	ASN	400	-7.040	-0.371	46.835	1.00	41.87
ATOM	2661	CB	ASN	400	-8.265	-0.971	47.538	1.00	46.04
ATOM	2662	CG	ASN	400	-9.575	-0.383	47.044	1.00	45.40
ATOM	2663	OD1	ASN	400	-10.103	-0.785	46.009	1.00	46.19
ATOM	2664	ND2	ASN	400	-10.118	0.567	47.800	1.00	45.31
ATOM	2665	C	ASN	400	-6.917	-0.953	45.422	1.00	43.13
ATOM	2666	O	ASN	400	-5.967	-0.562	44.708	1.00	38.80
ATOM	2667	C1	4040	1001	5.651	10.641	30.742	1.00	17.40
ATOM	2668	O1	4040	1001	4.293	10.841	30.577	1.00	20.93
ATOM	2669	N1	4040	1001	3.768	10.022	31.594	1.00	14.28
ATOM	2670	C4	4040	1001	4.658	9.392	32.346	1.00	11.79
ATOM	2671	C5	4040	1001	5.954	9.761	31.740	1.00	10.46
ATOM	2672	N2	4040	1001	8.425	9.939	31.690	1.00	2.00
ATOM	2673	C7	4040	1001	7.307	9.217	31.952	1.00	4.18
ATOM	2674	C16	4040	1001	7.364	7.912	32.368	1.00	2.00
ATOM	2675	C10	4040	1001	8.638	7.390	32.499	1.00	2.00
ATOM	2676	N5	4040	1001	9.698	8.129	32.226	1.00	8.25
ATOM	2677	C18	4040	1001	9.607	9.366	31.841	1.00	3.21
ATOM	2678	C15	4040	1001	4.715	7.838	35.779	1.00	4.77
ATOM	2679	C8	4040	1001	3.449	7.244	35.771	1.00	12.75
ATOM	2680	C17	4040	1001	2.585	7.298	34.670	1.00	12.33
ATOM	2681	C11	4040	1001	3.005	7.982	33.528	1.00	14.72
ATOM	2682	C13	4040	1001	4.278	8.594	33.526	1.00	16.11
ATOM	2683	C19	4040	1001	5.137	8.524	34.637	1.00	13.87
ATOM	2684	C2	4040	1001	6.629	11.300	29.783	1.00	18.40
ATOM	2685	N3	4040	1001	10.830	10.011	31.601	1.00	4.47
ATOM	2686	C6	4040	1001	10.987	10.898	30.601	1.00	6.40
ATOM	2687	C3	4040	1001	12.407	11.197	30.263	1.00	6.89
ATOM	2688	O4	4040	1001	10.094	11.460	29.962	1.00	16.54
ATOM	2689	OH2	TIP3	1	11.099	24.580	40.355	1.00	26.43
ATOM	2690	OH2	TIP3	2	16.034	17.889	35.924	1.00	21.43
ATOM	2691	OH2	TIP3	3	6.638	2.227	44.181	1.00	32.16
ATOM	2692	OH2	TIP3	4	20.438	1.594	42.414	1.00	32.35
ATOM	2693	OH2	TIP3	5	17.397	2.019	38.588	1.00	47.80
ATOM	2694	OH2	TIP3	6	21.365	7.894	38.349	1.00	53.39
ATOM	2695	OH2	TIP3	7	-16.615	14.917	35.305	1.00	39.74
ATOM	2696	OH2	TIP3	8	-19.383	15.176	34.969	1.00	34.63
ATOM	2697	OH2	TIP3	9	-2.647	9.079	29.753	1.00	21.81
ATOM	2698	OH2	TIP3	10	0.140	8.716	29.985	1.00	22.90
ATOM	2699	OH2	TIP3	11	-13.784	2.103	42.120	1.00	35.98
ATOM	2700	OH2	TIP3	12	0.565	-3.182	34.789	1.00	43.00
ATOM	2701	OH2	TIP3	13	0.462	-2.129	37.570	1.00	31.31
ATOM	2702	OH2	TIP3	14	11.861	-5.557	22.223	1.00	35.31
ATOM	2703	OH2	TIP3	15	6.133	-0.706	32.084	1.00	27.78
ATOM	2704	OH2	TIP3	16	-0.606	17.134	45.988	1.00	17.70
ATOM	2705	OH2	TIP3	17	10.025	15.635	16.157	1.00	43.57
ATOM	2706	OH2	TIP3	18	1.603	21.090	15.391	1.00	31.70
ATOM	2707	OH2	TIP3	19	-9.960	-0.572	11.478	1.00	12.99
ATOM	2708	OH2	TIP3	20	-3.898	11.090	10.729	1.00	35.00
ATOM	2709	OH2	TIP3	21	2.913	12.127	11.831	1.00	20.04
ATOM	2710	OH2	TIP3	22	-11.943	13.923	0.070	1.00	19.05
ATOM	2711	OH2	TIP3	23	-22.808	2.564	4.041	1.00	35.33
ATOM	2712	OH2	TIP3	24	8.047	7.521	-8.142	1.00	32.42

FIG. 1UU

```
ATOM   2713  OH2 TIP3   25     -16.704  19.733   2.447  1.00  18.06
ATOM   2714  OH2 TIP3   26     -19.392   7.013   8.226  1.00  26.38
ATOM   2715  OH2 TIP3   27      -2.939  14.818  -7.342  1.00  38.07
ATOM   2716  OH2 TIP3   28      18.620   3.235   3.927  1.00  31.48
ATOM   2717  OH2 TIP3   29      19.922  -2.960  -2.057  1.00  25.96
ATOM   2718  OH2 TIP3   30      23.569  -0.799  -6.475  1.00  42.59
ATOM   2719  OH2 TIP3   31     -14.080  -0.324   3.982  1.00  11.72
ATOM   2720  OH2 TIP3   32      -1.880 -10.669  10.357  1.00  36.98
ATOM   2721  OH2 TIP3   33      -3.231  -7.645   6.430  1.00  19.85
ATOM   2722  OH2 TIP3   34       2.195 -13.454  10.124  1.00  35.78
ATOM   2723  OH2 TIP3   35      -0.645 -13.187  10.089  1.00  19.79
ATOM   2724  OH2 TIP3   36       0.013 -10.801  22.565  1.00  30.67
ATOM   2725  OH2 TIP3   37       6.286  12.972  26.252  1.00  38.52
                          END
```

FIG. 2A

	Atom	Type	Resid	#	X	Y	Z	Occ	B
ATOM	1	N	ASP A	45	21.903	8.714	61.519	1.00	34.40
ATOM	2	CA	ASP A	45	21.423	9.997	62.113	1.00	36.18
ATOM	3	C	ASP A	45	20.751	10.818	61.005	1.00	33.68
ATOM	4	O	ASP A	45	19.516	10.888	60.905	1.00	33.15
ATOM	5	CB	ASP A	45	22.625	10.759	62.697	1.00	38.37
ATOM	6	CG	ASP A	45	22.249	11.690	63.845	1.00	39.28
ATOM	7	OD1	ASP A	45	21.044	11.989	64.033	1.00	40.07
ATOM	8	OD2	ASP A	45	23.181	12.121	64.563	1.00	39.46
ATOM	9	N	ASN A	46	21.576	11.411	60.150	1.00	31.22
ATOM	10	CA	ASN A	46	21.053	12.210	59.046	1.00	31.07
ATOM	11	C	ASN A	46	20.660	11.327	57.849	1.00	26.75
ATOM	12	O	ASN A	46	21.383	10.407	57.490	1.00	23.97
ATOM	13	CB	ASN A	46	22.087	13.258	58.623	1.00	33.86
ATOM	14	CG	ASN A	46	21.553	14.220	57.572	1.00	34.70
ATOM	15	OD1	ASN A	46	20.362	14.577	57.559	1.00	33.29
ATOM	16	ND2	ASN A	46	22.435	14.642	56.681	1.00	34.56
ATOM	17	N	GLN A	47	19.504	11.614	57.251	1.00	24.40
ATOM	18	CA	GLN A	47	18.998	10.857	56.101	1.00	23.13
ATOM	19	C	GLN A	47	19.964	10.849	54.902	1.00	20.34
ATOM	20	O	GLN A	47	19.770	10.084	53.962	1.00	21.47
ATOM	21	CB	GLN A	47	17.645	11.425	55.632	1.00	26.85
ATOM	22	CG	GLN A	47	16.471	11.410	56.641	1.00	30.76
ATOM	23	CD	GLN A	47	15.213	12.152	56.123	1.00	33.08
ATOM	24	OE1	GLN A	47	14.072	11.823	56.488	1.00	27.93
ATOM	25	NE2	GLN A	47	15.425	13.158	55.276	1.00	34.46
ATOM	26	N	PHE A	48	21.006	11.668	54.951	1.00	15.81
ATOM	27	CA	PHE A	48	21.959	11.773	53.859	1.00	15.50
ATOM	28	C	PHE A	48	23.318	11.257	54.197	1.00	17.92
ATOM	29	O	PHE A	48	23.602	10.946	55.343	1.00	26.00
ATOM	30	CB	PHE A	48	22.122	13.229	53.429	1.00	12.30
ATOM	31	CG	PHE A	48	20.835	13.880	53.069	1.00	12.37
ATOM	32	CD1	PHE A	48	20.014	14.361	54.047	1.00	9.42
ATOM	33	CD2	PHE A	48	20.413	13.941	51.755	1.00	14.72
ATOM	34	CE1	PHE A	48	18.804	14.882	53.751	1.00	9.25
ATOM	35	CE2	PHE A	48	19.175	14.471	51.434	1.00	12.23
ATOM	36	CZ	PHE A	48	18.370	14.938	52.442	1.00	11.80
ATOM	37	N	TYR A	49	24.158	11.165	53.177	1.00	16.03
ATOM	38	CA	TYR A	49	25.521	10.713	53.326	1.00	14.96
ATOM	39	C	TYR A	49	26.261	11.256	52.109	1.00	16.51
ATOM	40	O	TYR A	49	25.634	11.623	51.120	1.00	18.27
ATOM	41	CB	TYR A	49	25.579	9.179	53.444	1.00	16.48
ATOM	42	CG	TYR A	49	25.594	8.371	52.160	1.00	11.73
ATOM	43	CD1	TYR A	49	26.790	8.042	51.552	1.00	14.86
ATOM	44	CD2	TYR A	49	24.423	7.881	51.608	1.00	10.50
ATOM	45	CE1	TYR A	49	26.823	7.237	50.417	1.00	16.30
ATOM	46	CE2	TYR A	49	24.449	7.074	50.478	1.00	15.61
ATOM	47	CZ	TYR A	49	25.655	6.763	49.894	1.00	16.51
ATOM	48	OH	TYR A	49	25.702	5.998	48.768	1.00	22.01
ATOM	49	N	SER A	50	27.582	11.320	52.168	1.00	20.81
ATOM	50	CA	SER A	50	28.343	11.884	51.065	1.00	24.35
ATOM	51	C	SER A	50	29.404	10.963	50.489	1.00	26.61
ATOM	52	O	SER A	50	30.127	10.295	51.240	1.00	26.11
ATOM	53	CB	SER A	50	29.039	13.171	51.534	1.00	25.23
ATOM	54	OG	SER A	50	28.133	14.067	52.140	1.00	26.92
ATOM	55	N	VAL A	51	29.521	10.958	49.160	1.00	25.44
ATOM	56	CA	VAL A	51	30.538	10.144	48.506	1.00	27.28

FIG. 2B

ATOM	57	C	VAL	A	51	31.308	10.831	47.408	1.00	29.13
ATOM	58	O	VAL	A	51	30.775	11.655	46.669	1.00	28.02
ATOM	59	CB	VAL	A	51	30.026	8.784	47.960	1.00	25.85
ATOM	60	CG1	VAL	A	51	30.678	7.644	48.762	1.00	23.20
ATOM	61	CG2	VAL	A	51	28.508	8.712	47.981	1.00	22.29
ATOM	62	N	GLU	A	52	32.589	10.494	47.352	1.00	32.44
ATOM	63	CA	GLU	A	52	33.502	11.018	46.361	1.00	37.43
ATOM	64	C	GLU	A	52	33.277	10.302	45.019	1.00	41.03
ATOM	65	O	GLU	A	52	34.044	9.393	44.658	1.00	44.17
ATOM	66	CB	GLU	A	52	34.952	10.787	46.815	1.00	40.23
ATOM	67	CG	GLU	A	52	35.354	11.489	48.122	1.00	44.49
ATOM	68	CD	GLU	A	52	36.712	11.021	48.646	1.00	45.39
ATOM	69	OE1	GLU	A	52	37.699	11.075	47.886	1.00	46.92
ATOM	70	OE2	GLU	A	52	36.792	10.577	49.814	1.00	47.73
ATOM	71	N	VAL	A	53	32.211	10.676	44.306	1.00	39.71
ATOM	72	CA	VAL	A	53	31.918	10.099	42.992	1.00	36.87
ATOM	73	C	VAL	A	53	32.786	10.847	41.986	1.00	38.00
ATOM	74	O	VAL	A	53	32.397	11.899	41.459	1.00	36.09
ATOM	75	CB	VAL	A	53	30.435	10.252	42.576	1.00	34.18
ATOM	76	CG1	VAL	A	53	30.230	9.650	41.203	1.00	33.97
ATOM	77	CG2	VAL	A	53	29.524	9.566	43.571	1.00	28.11
ATOM	78	N	GLY	A	54	34.005	10.349	41.806	1.00	39.05
ATOM	79	CA	GLY	A	54	34.931	10.956	40.871	1.00	41.22
ATOM	80	C	GLY	A	54	35.621	12.226	41.322	1.00	42.09
ATOM	81	O	GLY	A	54	36.625	12.185	42.036	1.00	43.69
ATOM	82	N	ASP	A	55	35.111	13.357	40.847	1.00	42.82
ATOM	83	CA	ASP	A	55	35.690	14.659	41.166	1.00	44.27
ATOM	84	C	ASP	A	55	34.681	15.489	41.948	1.00	43.69
ATOM	85	O	ASP	A	55	34.921	16.665	42.244	1.00	44.83
ATOM	86	CB	ASP	A	55	36.056	15.392	39.862	1.00	44.71
ATOM	87	CG	ASP	A	55	37.208	16.379	40.034	1.00	45.70
ATOM	88	OD1	ASP	A	55	37.987	16.245	41.006	1.00	43.88
ATOM	89	OD2	ASP	A	55	37.345	17.278	39.173	1.00	45.77
ATOM	90	N	SER	A	56	33.546	14.869	42.264	1.00	41.87
ATOM	91	CA	SER	A	56	32.471	15.529	42.999	1.00	39.15
ATOM	92	C	SER	A	56	32.064	14.830	44.319	1.00	36.42
ATOM	93	O	SER	A	56	32.708	13.878	44.772	1.00	34.35
ATOM	94	CB	SER	A	56	31.255	15.715	42.070	1.00	40.76
ATOM	95	OG	SER	A	56	30.999	14.554	41.292	1.00	44.70
ATOM	96	N	THR	A	57	31.060	15.397	44.977	1.00	31.87
ATOM	97	CA	THR	A	57	30.531	14.855	46.211	1.00	28.23
ATOM	98	C	THR	A	57	29.044	14.683	45.999	1.00	26.15
ATOM	99	O	THR	A	57	28.341	15.636	45.741	1.00	28.09
ATOM	100	CB	THR	A	57	30.790	15.802	47.406	1.00	25.55
ATOM	101	OG1	THR	A	57	32.143	15.650	47.861	1.00	22.73
ATOM	102	CG2	THR	A	57	29.860	15.499	48.530	1.00	22.34
ATOM	103	N	PHE	A	58	28.561	13.463	46.135	1.00	26.71
ATOM	104	CA	PHE	A	58	27.148	13.206	45.925	1.00	27.96
ATOM	105	C	PHE	A	58	26.303	12.971	47.177	1.00	28.42
ATOM	106	O	PHE	A	58	25.740	11.892	47.379	1.00	34.14
ATOM	107	CB	PHE	A	58	26.963	12.040	44.960	1.00	24.54
ATOM	108	CG	PHE	A	58	26.701	12.457	43.533	1.00	20.20
ATOM	109	CD1	PHE	A	58	27.761	12.719	42.659	1.00	18.70
ATOM	110	CD2	PHE	A	58	25.394	12.511	43.051	1.00	17.72
ATOM	111	CE1	PHE	A	58	27.520	13.023	41.326	1.00	6.16
ATOM	112	CE2	PHE	A	58	25.143	12.816	41.716	1.00	6.65
ATOM	113	CZ	PHE	A	58	26.210	13.069	40.862	1.00	7.99
ATOM	114	N	THR	A	59	26.095	14.025	47.941	1.00	26.25
ATOM	115	CA	THR	A	59	25.305	13.932	49.153	1.00	20.51

FIG. 2C

ATOM	116	C	THR	A	59	23.921	13.489	48.769	1.00	18.74
ATOM	117	O	THR	A	59	23.123	14.273	48.293	1.00	20.15
ATOM	118	CB	THR	A	59	25.244	15.284	49.863	1.00	18.08
ATOM	119	OG1	THR	A	59	26.585	15.707	50.146	1.00	17.42
ATOM	120	CG2	THR	A	59	24.450	15.190	51.151	1.00	17.08
ATOM	121	N	VAL	A	60	23.647	12.208	48.953	1.00	17.47
ATOM	122	CA	VAL	A	60	22.344	11.668	48.611	1.00	15.56
ATOM	123	C	VAL	A	60	21.676	10.974	49.764	1.00	9.70
ATOM	124	O	VAL	A	60	22.300	10.636	50.742	1.00	11.46
ATOM	125	CB	VAL	A	60	22.447	10.666	47.399	1.00	17.14
ATOM	126	CG1	VAL	A	60	22.985	11.395	46.174	1.00	16.49
ATOM	127	CG2	VAL	A	60	23.379	9.471	47.739	1.00	13.46
ATOM	128	N	LEU	A	61	20.380	10.780	49.637	1.00	12.17
ATOM	129	CA	LEU	A	61	19.609	10.070	50.642	1.00	19.00
ATOM	130	C	LEU	A	61	20.217	8.665	50.711	1.00	21.44
ATOM	131	O	LEU	A	61	20.570	8.091	49.680	1.00	24.40
ATOM	132	CB	LEU	A	61	18.130	9.991	50.207	1.00	17.94
ATOM	133	CG	LEU	A	61	17.263	11.258	50.276	1.00	16.60
ATOM	134	CD1	LEU	A	61	16.002	11.052	49.448	1.00	13.63
ATOM	135	CD2	LEU	A	61	16.908	11.606	51.740	1.00	16.01
ATOM	136	N	LYS	A	62	20.357	8.127	51.917	1.00	23.01
ATOM	137	CA	LYS	A	62	20.951	6.803	52.133	1.00	21.23
ATOM	138	C	LYS	A	62	20.420	5.611	51.334	1.00	19.20
ATOM	139	O	LYS	A	62	21.134	4.627	51.177	1.00	17.05
ATOM	140	CB	LYS	A	62	20.926	6.471	53.627	1.00	22.99
ATOM	141	CG	LYS	A	62	22.037	7.137	54.381	1.00	21.04
ATOM	142	CD	LYS	A	62	21.743	7.287	55.857	1.00	23.25
ATOM	143	CE	LYS	A	62	22.916	8.006	56.539	1.00	23.94
ATOM	144	NZ	LYS	A	62	22.712	8.217	58.005	1.00	20.22
ATOM	145	N	ARG	A	63	19.167	5.677	50.877	1.00	17.63
ATOM	146	CA	ARG	A	63	18.548	4.610	50.083	1.00	17.67
ATOM	147	C	ARG	A	63	19.300	4.304	48.780	1.00	20.60
ATOM	148	O	ARG	A	63	19.006	3.288	48.146	1.00	25.79
ATOM	149	CB	ARG	A	63	17.097	4.968	49.745	1.00	13.35
ATOM	150	CG	ARG	A	63	16.953	6.318	49.069	1.00	11.45
ATOM	151	CD	ARG	A	63	15.512	6.740	48.897	1.00	7.72
ATOM	152	NE	ARG	A	63	14.811	5.884	47.963	1.00	6.68
ATOM	153	CZ	ARG	A	63	13.529	6.005	47.671	1.00	7.81
ATOM	154	NH1	ARG	A	63	12.801	6.944	48.229	1.00	13.19
ATOM	155	NH2	ARG	A	63	12.949	5.152	46.851	1.00	13.87
ATOM	156	N	TYR	A	64	20.246	5.173	48.385	1.00	21.13
ATOM	157	CA	TYR	A	64	21.052	5.010	47.167	1.00	16.30
ATOM	158	C	TYR	A	64	22.460	4.551	47.539	1.00	17.65
ATOM	159	O	TYR	A	64	23.174	5.215	48.283	1.00	19.10
ATOM	160	CB	TYR	A	64	21.081	6.313	46.378	1.00	12.30
ATOM	161	CG	TYR	A	64	19.691	6.834	46.090	1.00	7.10
ATOM	162	CD1	TYR	A	64	18.815	6.113	45.281	1.00	6.87
ATOM	163	CD2	TYR	A	64	19.235	8.040	46.643	1.00	5.16
ATOM	164	CE1	TYR	A	64	17.521	6.572	45.031	1.00	2.99
ATOM	165	CE2	TYR	A	64	17.932	8.507	46.391	1.00	3.57
ATOM	166	CZ	TYR	A	64	17.079	7.767	45.584	1.00	5.43
ATOM	167	OH	TYR	A	64	15.773	8.195	45.320	1.00	6.01
ATOM	168	N	GLN	A	65	22.820	3.364	47.064	1.00	20.73
ATOM	169	CA	GLN	A	65	24.095	2.737	47.370	1.00	18.99
ATOM	170	C	GLN	A	65	24.882	2.428	46.124	1.00	19.39
ATOM	171	O	GLN	A	65	24.353	2.438	45.037	1.00	23.28
ATOM	172	CB	GLN	A	65	23.824	1.442	48.110	1.00	23.17
ATOM	173	CG	GLN	A	65	22.951	1.663	49.337	1.00	26.90
ATOM	174	CD	GLN	A	65	21.666	0.843	49.324	1.00	33.61

FIG. 2D

ATOM	175	OE1	GLN	A	65	20.649	1.243	48.714	1.00	37.34
ATOM	176	NE2	GLN	A	65	21.690	-0.306	50.016	1.00	29.61
ATOM	177	N	ASN	A	66	26.155	2.131	46.303	1.00	20.73
ATOM	178	CA	ASN	A	66	27.040	1.837	45.205	1.00	22.18
ATOM	179	C	ASN	A	66	26.912	2.829	44.044	1.00	23.64
ATOM	180	O	ASN	A	66	26.592	2.442	42.915	1.00	21.80
ATOM	181	CB	ASN	A	66	26.807	0.423	44.711	1.00	23.36
ATOM	182	CG	ASN	A	66	28.104	-0.320	44.454	1.00	23.74
ATOM	183	OD1	ASN	A	66	28.102	-1.548	44.360	1.00	30.68
ATOM	184	ND2	ASN	A	66	29.217	0.400	44.365	1.00	19.97
ATOM	185	N	LEU	A	67	27.195	4.105	44.329	1.00	26.13
ATOM	186	CA	LEU	A	67	27.125	5.169	43.321	1.00	26.96
ATOM	187	C	LEU	A	67	28.303	5.048	42.370	1.00	27.05
ATOM	188	O	LEU	A	67	29.454	4.966	42.806	1.00	23.63
ATOM	189	CB	LEU	A	67	27.167	6.560	43.963	1.00	27.02
ATOM	190	CG	LEU	A	67	26.214	6.979	45.083	1.00	26.97
ATOM	191	CD1	LEU	A	67	25.953	8.482	44.896	1.00	23.30
ATOM	192	CD2	LEU	A	67	24.905	6.196	45.058	1.00	22.27
ATOM	193	N	LYS	A	68	28.012	5.049	41.075	1.00	27.57
ATOM	194	CA	LYS	A	68	29.052	4.935	40.063	1.00	27.90
ATOM	195	C	LYS	A	68	28.769	6.004	39.015	1.00	26.86
ATOM	196	O	LYS	A	68	27.631	6.206	38.628	1.00	29.53
ATOM	197	CB	LYS	A	68	29.002	3.532	39.445	1.00	31.18
ATOM	198	CG	LYS	A	68	30.135	3.254	38.466	1.00	41.51
ATOM	199	CD	LYS	A	68	30.117	1.819	37.930	1.00	45.53
ATOM	200	CE	LYS	A	68	31.469	1.443	37.291	1.00	48.89
ATOM	201	NZ	LYS	A	68	31.615	-0.040	37.036	1.00	50.37
ATOM	202	N	PRO	A	69	29.804	6.701	38.539	1.00	27.17
ATOM	203	CA	PRO	A	69	29.622	7.756	37.532	1.00	26.52
ATOM	204	C	PRO	A	69	29.270	7.270	36.140	1.00	25.11
ATOM	205	O	PRO	A	69	29.877	6.336	35.617	1.00	25.86
ATOM	206	CB	PRO	A	69	30.989	8.443	37.511	1.00	26.89
ATOM	207	CG	PRO	A	69	31.938	7.293	37.725	1.00	28.83
ATOM	208	CD	PRO	A	69	31.231	6.524	38.863	1.00	28.51
ATOM	209	N	ILE	A	70	28.259	7.899	35.556	1.00	24.95
ATOM	210	CA	ILE	A	70	27.845	7.586	34.202	1.00	25.17
ATOM	211	C	ILE	A	70	27.639	8.877	33.415	1.00	26.56
ATOM	212	O	ILE	A	70	28.656	9.620	33.256	1.00	26.71
ATOM	213	CB	ILE	A	70	26.571	6.732	34.181	1.00	26.02
ATOM	214	CG1	ILE	A	70	25.377	7.530	34.653	1.00	24.95
ATOM	215	CG2	ILE	A	70	26.747	5.528	35.114	1.00	32.72
ATOM	216	CD1	ILE	A	70	24.131	6.680	34.823	1.00	26.64
ATOM	217	N	GLY	A	73	29.035	15.317	33.639	1.00	45.08
ATOM	218	CA	GLY	A	73	28.781	16.123	32.424	1.00	45.96
ATOM	219	C	GLY	A	73	28.701	17.625	32.656	1.00	47.11
ATOM	220	O	GLY	A	73	28.688	18.097	33.804	1.00	47.57
ATOM	221	N	ALA	A	74	28.619	18.359	31.544	1.00	46.79
ATOM	222	CA	ALA	A	74	28.545	19.825	31.525	1.00	45.55
ATOM	223	C	ALA	A	74	27.288	20.405	32.169	1.00	44.71
ATOM	224	O	ALA	A	74	27.337	21.484	32.763	1.00	44.95
ATOM	225	CB	ALA	A	74	28.685	20.340	30.092	1.00	46.21
ATOM	226	N	GLN	A	75	26.154	19.721	32.031	1.00	42.77
ATOM	227	CA	GLN	A	75	24.920	20.209	32.648	1.00	42.40
ATOM	228	C	GLN	A	75	24.456	19.391	33.880	1.00	40.14
ATOM	229	O	GLN	A	75	23.268	19.350	34.229	1.00	41.54
ATOM	230	CB	GLN	A	75	23.819	20.353	31.596	1.00	41.18
ATOM	231	CG	GLN	A	75	23.758	19.231	30.590	1.00	42.08
ATOM	232	CD	GLN	A	75	22.721	18.190	30.950	1.00	44.75
ATOM	233	OE1	GLN	A	75	23.036	17.003	31.044	1.00	46.19

FIG. 2E

ATOM	234	NE2	GLN	A	75	21.472	18.630	31.148	1.00	43.10
ATOM	235	N	GLY	A	76	25.427	18.818	34.585	1.00	36.77
ATOM	236	CA	GLY	A	76	25.122	18.032	35.756	1.00	32.12
ATOM	237	C	GLY	A	76	25.867	16.726	35.649	1.00	29.10
ATOM	238	O	GLY	A	76	26.264	16.315	34.568	1.00	28.74
ATOM	239	N	ILE	A	77	26.126	16.107	36.791	1.00	29.23
ATOM	240	CA	ILE	A	77	26.826	14.831	36.830	1.00	26.79
ATOM	241	C	ILE	A	77	25.793	13.741	37.052	1.00	23.44
ATOM	242	O	ILE	A	77	24.843	13.928	37.808	1.00	22.33
ATOM	243	CB	ILE	A	77	27.894	14.797	37.949	1.00	28.83
ATOM	244	CG1	ILE	A	77	28.438	16.221	38.246	1.00	30.10
ATOM	245	CG2	ILE	A	77	28.991	13.796	37.571	1.00	23.11
ATOM	246	CD1	ILE	A	77	28.853	17.081	37.009	1.00	30.30
ATOM	247	N	VAL	A	78	25.932	12.632	36.335	1.00	20.94
ATOM	248	CA	VAL	A	78	24.982	11.534	36.467	1.00	19.24
ATOM	249	C	VAL	A	78	25.671	10.326	37.115	1.00	17.37
ATOM	250	O	VAL	A	78	26.851	10.069	36.884	1.00	14.75
ATOM	251	CB	VAL	A	78	24.352	11.159	35.088	1.00	18.14
ATOM	252	CG1	VAL	A	78	23.139	10.244	35.275	1.00	19.05
ATOM	253	CG2	VAL	A	78	23.926	12.422	34.357	1.00	19.83
ATOM	254	N	CYS	A	79	24.922	9.618	37.954	1.00	16.64
ATOM	255	CA	CYS	A	79	25.417	8.453	38.681	1.00	16.84
ATOM	256	C	CYS	A	79	24.441	7.314	38.618	1.00	14.35
ATOM	257	O	CYS	A	79	23.231	7.516	38.538	1.00	15.11
ATOM	258	CB	CYS	A	79	25.643	8.780	40.166	1.00	16.44
ATOM	259	SG	CYS	A	79	27.336	9.176	40.532	1.00	30.72
ATOM	260	N	ALA	A	80	24.987	6.108	38.571	1.00	14.50
ATOM	261	CA	ALA	A	80	24.177	4.900	38.582	1.00	17.43
ATOM	262	C	ALA	A	80	24.150	4.520	40.066	1.00	15.98
ATOM	263	O	ALA	A	80	25.122	4.761	40.795	1.00	16.01
ATOM	264	CB	ALA	A	80	24.849	3.795	37.763	1.00	14.56
ATOM	265	N	ALA	A	81	23.038	3.966	40.527	1.00	16.06
ATOM	266	CA	ALA	A	81	22.962	3.573	41.920	1.00	15.59
ATOM	267	C	ALA	A	81	21.836	2.609	42.147	1.00	15.48
ATOM	268	O	ALA	A	81	20.914	2.498	41.323	1.00	15.11
ATOM	269	CB	ALA	A	81	22.775	4.791	42.814	1.00	12.88
ATOM	270	N	TYR	A	82	21.926	1.933	43.297	1.00	18.71
ATOM	271	CA	TYR	A	82	20.930	0.961	43.765	1.00	16.44
ATOM	272	C	TYR	A	82	20.013	1.596	44.823	1.00	14.14
ATOM	273	O	TYR	A	82	20.476	2.140	45.800	1.00	14.37
ATOM	274	CB	TYR	A	82	21.641	-0.273	44.354	1.00	15.08
ATOM	275	CG	TYR	A	82	20.690	-1.255	45.001	1.00	16.38
ATOM	276	CD1	TYR	A	82	19.617	-1.782	44.288	1.00	13.31
ATOM	277	CD2	TYR	A	82	20.809	-1.592	46.352	1.00	14.38
ATOM	278	CE1	TYR	A	82	18.684	-2.597	44.903	1.00	16.69
ATOM	279	CE2	TYR	A	82	19.867	-2.408	46.973	1.00	9.96
ATOM	280	CZ	TYR	A	82	18.809	-2.891	46.253	1.00	11.01
ATOM	281	OH	TYR	A	82	17.791	-3.550	46.886	1.00	10.41
ATOM	282	N	ASP	A	83	18.713	1.517	44.623	1.00	15.81
ATOM	283	CA	ASP	A	83	17.777	2.073	45.567	1.00	15.84
ATOM	284	C	ASP	A	83	17.200	0.958	46.418	1.00	16.76
ATOM	285	O	ASP	A	83	16.277	0.256	46.004	1.00	13.18
ATOM	286	CB	ASP	A	83	16.647	2.802	44.838	1.00	17.74
ATOM	287	CG	ASP	A	83	15.647	3.428	45.786	1.00	19.13
ATOM	288	OD1	ASP	A	83	14.588	3.863	45.315	1.00	22.66
ATOM	289	OD2	ASP	A	83	15.914	3.500	46.997	1.00	23.77
ATOM	290	N	ALA	A	84	17.697	0.876	47.645	1.00	16.89
ATOM	291	CA	ALA	A	84	17.280	-0.126	48.609	1.00	14.73
ATOM	292	C	ALA	A	84	15.804	-0.079	48.879	1.00	13.83

FIG. 2F

ATOM	293	O	ALA	A	84	15.166	-1.115	49.071	1.00	18.36
ATOM	294	CB	ALA	A	84	18.055	0.049	49.872	1.00	15.67
ATOM	295	N	VAL	A	85	15.229	1.107	48.818	1.00	13.99
ATOM	296	CA	VAL	A	85	13.815	1.235	49.074	1.00	13.29
ATOM	297	C	VAL	A	85	12.962	0.722	47.926	1.00	19.89
ATOM	298	O	VAL	A	85	11.956	0.041	48.142	1.00	24.83
ATOM	299	CB	VAL	A	85	13.440	2.694	49.366	1.00	11.26
ATOM	300	CG1	VAL	A	85	11.928	2.839	49.531	1.00	8.90
ATOM	301	CG2	VAL	A	85	14.186	3.165	50.597	1.00	9.72
ATOM	302	N	LEU	A	86	13.373	1.011	46.696	1.00	22.18
ATOM	303	CA	LEU	A	86	12.579	0.598	45.548	1.00	20.84
ATOM	304	C	LEU	A	86	13.108	-0.720	45.005	1.00	20.77
ATOM	305	O	LEU	A	86	12.406	-1.382	44.256	1.00	24.37
ATOM	306	CB	LEU	A	86	12.634	1.692	44.481	1.00	20.31
ATOM	307	CG	LEU	A	86	11.450	2.248	43.687	1.00	18.86
ATOM	308	CD1	LEU	A	86	10.348	2.823	44.545	1.00	19.36
ATOM	309	CD2	LEU	A	86	12.019	3.330	42.829	1.00	15.44
ATOM	310	N	ASP	A	87	14.311	-1.113	45.427	1.00	19.59
ATOM	311	CA	ASP	A	87	14.952	-2.360	44.991	1.00	24.37
ATOM	312	C	ASP	A	87	15.287	-2.340	43.495	1.00	27.94
ATOM	313	O	ASP	A	87	15.411	-3.393	42.852	1.00	30.01
ATOM	314	CB	ASP	A	87	14.030	-3.558	45.301	1.00	23.50
ATOM	315	CG	ASP	A	87	14.741	-4.908	45.226	1.00	20.28
ATOM	316	OD1	ASP	A	87	15.985	-4.965	45.357	1.00	18.88
ATOM	317	OD2	ASP	A	87	14.030	-5.924	45.052	1.00	20.73
ATOM	318	N	ARG	A	88	15.390	-1.132	42.947	1.00	27.96
ATOM	319	CA	ARG	A	88	15.695	-0.918	41.535	1.00	24.53
ATOM	320	C	ARG	A	88	17.006	-0.164	41.452	1.00	22.72
ATOM	321	O	ARG	A	88	17.534	0.272	42.465	1.00	21.23
ATOM	322	CB	ARG	A	88	14.601	-0.058	40.884	1.00	26.06
ATOM	323	CG	ARG	A	88	13.243	-0.708	40.833	1.00	31.50
ATOM	324	CD	ARG	A	88	12.104	0.309	40.666	1.00	37.98
ATOM	325	NE	ARG	A	88	12.189	1.086	39.426	1.00	44.46
ATOM	326	CZ	ARG	A	88	11.270	1.970	39.018	1.00	47.83
ATOM	327	NH1	ARG	A	88	10.176	2.189	39.746	1.00	46.37
ATOM	328	NH2	ARG	A	88	11.452	2.659	37.886	1.00	46.81
ATOM	329	N	ASN	A	89	17.584	-0.121	40.257	1.00	21.96
ATOM	330	CA	ASN	A	89	18.799	0.635	40.015	1.00	17.98
ATOM	331	C	ASN	A	89	18.171	1.862	39.394	1.00	17.64
ATOM	332	O	ASN	A	89	17.225	1.736	38.610	1.00	16.27
ATOM	333	CB	ASN	A	89	19.669	-0.033	38.976	1.00	21.06
ATOM	334	CG	ASN	A	89	20.241	-1.324	39.448	1.00	22.14
ATOM	335	OD1	ASN	A	89	21.295	-1.353	40.064	1.00	24.48
ATOM	336	ND2	ASN	A	89	19.564	-2.413	39.142	1.00	24.86
ATOM	337	N	VAL	A	90	18.655	3.042	39.787	1.00	16.48
ATOM	338	CA	VAL	A	90	18.138	4.317	39.303	1.00	8.72
ATOM	339	C	VAL	A	90	19.312	5.100	38.821	1.00	7.86
ATOM	340	O	VAL	A	90	20.446	4.734	39.066	1.00	6.68
ATOM	341	CB	VAL	A	90	17.506	5.169	40.433	1.00	8.10
ATOM	342	CG1	VAL	A	90	16.307	4.488	41.040	1.00	7.17
ATOM	343	CG2	VAL	A	90	18.555	5.489	41.511	1.00	8.82
ATOM	344	N	ALA	A	91	19.025	6.207	38.145	1.00	10.32
ATOM	345	CA	ALA	A	91	20.064	7.112	37.641	1.00	14.10
ATOM	346	C	ALA	A	91	19.824	8.402	38.409	1.00	10.46
ATOM	347	O	ALA	A	91	18.677	8.815	38.552	1.00	10.39
ATOM	348	CB	ALA	A	91	19.911	7.349	36.127	1.00	11.77
ATOM	349	N	ILE	A	92	20.888	8.967	38.977	1.00	13.28
ATOM	350	CA	ILE	A	92	20.811	10.215	39.756	1.00	14.22
ATOM	351	C	ILE	A	92	21.681	11.322	39.153	1.00	10.61

FIG. 2G

ATOM	352	O	ILE	A	92	22.872	11.142	38.980	1.00	9.03
ATOM	353	CB	ILE	A	92	21.312	10.010	41.221	1.00	17.15
ATOM	354	CG1	ILE	A	92	20.709	8.742	41.845	1.00	16.75
ATOM	355	CG2	ILE	A	92	20.994	11.260	42.062	1.00	13.54
ATOM	356	CD1	ILE	A	92	21.240	8.459	43.256	1.00	20.93
ATOM	357	N	LYS	A	93	21.095	12.483	38.889	1.00	14.77
ATOM	358	CA	LYS	A	93	21.851	13.604	38.327	1.00	12.79
ATOM	359	C	LYS	A	93	21.946	14.804	39.309	1.00	9.97
ATOM	360	O	LYS	A	93	20.943	15.280	39.825	1.00	11.17
ATOM	361	CB	LYS	A	93	21.203	14.056	37.019	1.00	14.33
ATOM	362	CG	LYS	A	93	21.917	15.238	36.389	1.00	18.76
ATOM	363	CD	LYS	A	93	21.078	15.917	35.332	1.00	23.53
ATOM	364	CE	LYS	A	93	21.054	15.110	34.067	1.00	22.04
ATOM	365	NZ	LYS	A	93	20.001	15.633	33.164	1.00	28.29
ATOM	366	N	LYS	A	94	23.154	15.298	39.533	1.00	10.00
ATOM	367	CA	LYS	A	94	23.388	16.427	40.425	1.00	11.97
ATOM	368	C	LYS	A	94	23.396	17.765	39.688	1.00	13.01
ATOM	369	O	LYS	A	94	24.211	17.978	38.794	1.00	8.56
ATOM	370	CB	LYS	A	94	24.756	16.268	41.106	1.00	9.16
ATOM	371	CG	LYS	A	94	25.102	17.296	42.205	1.00	5.83
ATOM	372	CD	LYS	A	94	26.621	17.217	42.451	1.00	4.53
ATOM	373	CE	LYS	A	94	27.109	18.149	43.574	1.00	7.98
ATOM	374	NZ	LYS	A	94	28.612	18.218	43.640	1.00	4.59
ATOM	375	N	LEU	A	95	22.481	18.653	40.077	1.00	17.90
ATOM	376	CA	LEU	A	95	22.395	20.013	39.530	1.00	17.86
ATOM	377	C	LEU	A	95	23.158	20.951	40.488	1.00	16.55
ATOM	378	O	LEU	A	95	22.586	21.431	41.449	1.00	20.96
ATOM	379	CB	LEU	A	95	20.926	20.486	39.432	1.00	18.23
ATOM	380	CG	LEU	A	95	20.238	20.496	38.065	1.00	12.58
ATOM	381	CD1	LEU	A	95	20.349	19.122	37.454	1.00	14.99
ATOM	382	CD2	LEU	A	95	18.786	20.976	38.161	1.00	5.98
ATOM	383	N	SER	A	96	24.449	21.168	40.257	1.00	17.33
ATOM	384	CA	SER	A	96	25.250	22.042	41.103	1.00	21.25
ATOM	385	C	SER	A	96	24.932	23.521	40.877	1.00	23.71
ATOM	386	O	SER	A	96	25.244	24.083	39.811	1.00	24.71
ATOM	387	CB	SER	A	96	26.737	21.817	40.848	1.00	19.80
ATOM	388	OG	SER	A	96	27.057	20.438	40.793	1.00	25.39
ATOM	389	N	ARG	A	97	24.358	24.154	41.903	1.00	24.38
ATOM	390	CA	ARG	A	97	24.007	25.566	41.831	1.00	24.92
ATOM	391	C	ARG	A	97	23.288	25.770	40.511	1.00	25.58
ATOM	392	O	ARG	A	97	23.861	26.317	39.579	1.00	29.24
ATOM	393	CB	ARG	A	97	25.280	26.410	41.829	1.00	22.33
ATOM	394	CG	ARG	A	97	26.001	26.460	43.136	1.00	23.30
ATOM	395	CD	ARG	A	97	25.280	27.362	44.068	1.00	23.60
ATOM	396	NE	ARG	A	97	26.226	28.057	44.926	1.00	27.02
ATOM	397	CZ	ARG	A	97	25.915	29.072	45.719	1.00	22.30
ATOM	398	NH1	ARG	A	97	24.676	29.536	45.768	1.00	19.93
ATOM	399	NH2	ARG	A	97	26.841	29.561	46.529	1.00	29.55
ATOM	400	N	PRO	A	98	22.061	25.248	40.384	1.00	24.73
ATOM	401	CA	PRO	A	98	21.325	25.409	39.119	1.00	24.14
ATOM	402	C	PRO	A	98	20.880	26.875	38.814	1.00	26.34
ATOM	403	O	PRO	A	98	20.656	27.265	37.645	1.00	27.05
ATOM	404	CB	PRO	A	98	20.142	24.450	39.296	1.00	21.07
ATOM	405	CG	PRO	A	98	19.915	24.461	40.811	1.00	20.34
ATOM	406	CD	PRO	A	98	21.310	24.439	41.361	1.00	20.62
ATOM	407	N	PHE	A	99	20.810	27.685	39.864	1.00	25.58
ATOM	408	CA	PHE	A	99	20.404	29.079	39.786	1.00	22.88
ATOM	409	C	PHE	A	99	21.628	29.978	39.658	1.00	23.17
ATOM	410	O	PHE	A	99	21.511	31.186	39.871	1.00	27.58

FIG. 2H

ATOM	411	CB	PHE	A	99	19.701	29.418	41.073	1.00	19.95
ATOM	412	CG	PHE	A	99	20.410	28.882	42.262	1.00	24.21
ATOM	413	CD1	PHE	A	99	19.984	27.698	42.866	1.00	25.78
ATOM	414	CD2	PHE	A	99	21.579	29.480	42.698	1.00	23.29
ATOM	415	CE1	PHE	A	99	20.708	27.127	43.894	1.00	26.74
ATOM	416	CE2	PHE	A	99	22.319	28.929	43.723	1.00	27.03
ATOM	417	CZ	PHE	A	99	21.893	27.736	44.320	1.00	26.84
ATOM	418	N	GLN	A	100	22.790	29.411	39.329	1.00	20.86
ATOM	419	CA	GLN	A	100	23.998	30.196	39.203	1.00	19.24
ATOM	420	C	GLN	A	100	23.933	31.238	38.081	1.00	23.28
ATOM	421	O	GLN	A	100	24.648	32.240	38.123	1.00	23.81
ATOM	422	CB	GLN	A	100	25.228	29.309	39.086	1.00	16.82
ATOM	423	CG	GLN	A	100	25.359	28.536	37.827	1.00	16.73
ATOM	424	CD	GLN	A	100	26.782	28.575	37.334	1.00	20.50
ATOM	425	OE1	GLN	A	100	27.087	29.215	36.325	1.00	29.92
ATOM	426	NE2	GLN	A	100	27.674	27.945	38.062	1.00	21.47
ATOM	427	N	ASN	A	101	23.110	30.972	37.064	1.00	23.78
ATOM	428	CA	ASN	A	101	22.879	31.892	35.958	1.00	18.93
ATOM	429	C	ASN	A	101	21.527	31.586	35.318	1.00	19.15
ATOM	430	O	ASN	A	101	20.894	30.576	35.635	1.00	16.93
ATOM	431	CB	ASN	A	101	24.078	32.051	34.981	1.00	19.19
ATOM	432	CG	ASN	A	101	24.403	30.812	34.145	1.00	19.46
ATOM	433	OD1	ASN	A	101	23.556	30.291	33.428	1.00	23.89
ATOM	434	ND2	ASN	A	101	25.670	30.417	34.146	1.00	15.74
ATOM	435	N	GLN	A	102	21.022	32.521	34.523	1.00	21.89
ATOM	436	CA	GLN	A	102	19.701	32.356	33.922	1.00	23.21
ATOM	437	C	GLN	A	102	19.533	31.258	32.888	1.00	22.40
ATOM	438	O	GLN	A	102	18.412	30.837	32.617	1.00	21.56
ATOM	439	CB	GLN	A	102	19.199	33.682	33.361	1.00	29.90
ATOM	440	CG	GLN	A	102	19.154	34.804	34.390	1.00	31.93
ATOM	441	CD	GLN	A	102	18.372	36.001	33.894	1.00	34.84
ATOM	442	OE1	GLN	A	102	17.132	35.990	33.899	1.00	36.18
ATOM	443	NE2	GLN	A	102	19.090	37.040	33.437	1.00	33.10
ATOM	444	N	THR	A	103	20.634	30.821	32.289	1.00	22.92
ATOM	445	CA	THR	A	103	20.591	29.745	31.312	1.00	24.22
ATOM	446	C	THR	A	103	20.342	28.483	32.154	1.00	23.67
ATOM	447	O	THR	A	103	19.277	27.882	32.069	1.00	26.93
ATOM	448	CB	THR	A	103	21.934	29.672	30.553	1.00	27.86
ATOM	449	OG1	THR	A	103	22.235	30.966	29.994	1.00	24.55
ATOM	450	CG2	THR	A	103	21.871	28.622	29.427	1.00	28.78
ATOM	451	N	HIS	A	104	21.292	28.141	33.024	1.00	25.35
ATOM	452	CA	HIS	A	104	21.158	27.002	33.947	1.00	23.26
ATOM	453	C	HIS	A	104	19.839	27.086	34.677	1.00	20.46
ATOM	454	O	HIS	A	104	19.115	26.113	34.763	1.00	24.89
ATOM	455	CB	HIS	A	104	22.237	27.041	35.044	1.00	23.44
ATOM	456	CG	HIS	A	104	23.612	26.709	34.567	1.00	22.14
ATOM	457	ND1	HIS	A	104	23.912	25.515	33.950	1.00	27.61
ATOM	458	CD2	HIS	A	104	24.775	27.388	34.648	1.00	23.89
ATOM	459	CE1	HIS	A	104	25.201	25.472	33.674	1.00	21.83
ATOM	460	NE2	HIS	A	104	25.748	26.597	34.087	1.00	21.86
ATOM	461	N	ALA	A	105	19.506	28.277	35.156	1.00	18.99
ATOM	462	CA	ALA	A	105	18.295	28.469	35.941	1.00	16.67
ATOM	463	C	ALA	A	105	16.977	28.389	35.226	1.00	15.43
ATOM	464	O	ALA	A	105	15.984	27.969	35.814	1.00	15.84
ATOM	465	CB	ALA	A	105	18.391	29.746	36.724	1.00	19.42
ATOM	466	N	LYS	A	106	16.923	28.806	33.970	1.00	18.41
ATOM	467	CA	LYS	A	106	15.614	28.748	33.312	1.00	20.15
ATOM	468	C	LYS	A	106	15.360	27.366	32.720	1.00	18.69
ATOM	469	O	LYS	A	106	14.232	26.949	32.474	1.00	20.92

FIG. 2I

ATOM	470	CB	LYS	A	106	15.590	29.792	32.202	1.00	23.44
ATOM	471	CG	LYS	A	106	14.173	30.098	31.717	1.00	27.12
ATOM	472	CD	LYS	A	106	14.060	31.508	31.132	1.00	33.79
ATOM	473	CE	LYS	A	106	15.141	31.794	30.090	1.00	35.65
ATOM	474	NZ	LYS	A	106	14.827	31.086	28.854	1.00	35.14
ATOM	475	N	ARG	A	107	16.477	26.670	32.441	1.00	19.73
ATOM	476	CA	ARG	A	107	16.392	25.293	31.985	1.00	19.95
ATOM	477	C	ARG	A	107	16.047	24.354	33.148	1.00	18.65
ATOM	478	O	ARG	A	107	15.202	23.476	33.053	1.00	17.46
ATOM	479	CB	ARG	A	107	17.754	24.918	31.383	1.00	22.01
ATOM	480	CG	ARG	A	107	18.130	23.452	31.608	1.00	30.96
ATOM	481	CD	ARG	A	107	19.475	23.098	30.938	1.00	39.76
ATOM	482	NE	ARG	A	107	19.261	22.209	29.788	1.00	43.62
ATOM	483	CZ	ARG	A	107	20.326	21.919	29.013	1.00	45.78
ATOM	484	NH1	ARG	A	107	21.516	22.423	29.297	1.00	43.52
ATOM	485	NH2	ARG	A	107	20.170	21.115	27.957	1.00	46.85
ATOM	486	N	ALA	A	108	16.771	24.554	34.265	1.00	16.31
ATOM	487	CA	ALA	A	108	16.500	23.766	35.467	1.00	16.08
ATOM	488	C	ALA	A	108	15.036	23.886	35.919	1.00	18.41
ATOM	489	O	ALA	A	108	14.317	22.907	36.070	1.00	22.63
ATOM	490	CB	ALA	A	108	17.430	24.262	36.580	1.00	14.86
ATOM	491	N	TYR	A	109	14.616	25.143	36.183	1.00	16.47
ATOM	492	CA	TYR	A	109	13.242	25.374	36.642	1.00	16.30
ATOM	493	C	TYR	A	109	12.210	24.806	35.658	1.00	16.15
ATOM	494	O	TYR	A	109	11.180	24.267	36.041	1.00	13.54
ATOM	495	CB	TYR	A	109	13.042	26.888	36.802	1.00	20.39
ATOM	496	CG	TYR	A	109	11.659	27.186	37.284	1.00	25.65
ATOM	497	CD1	TYR	A	109	11.298	26.891	38.598	1.00	25.78
ATOM	498	CD2	TYR	A	109	10.728	27.786	36.433	1.00	26.01
ATOM	499	CE1	TYR	A	109	10.021	27.191	39.057	1.00	24.75
ATOM	500	CE2	TYR	A	109	9.452	28.087	36.892	1.00	26.22
ATOM	501	CZ	TYR	A	109	9.097	27.792	38.196	1.00	27.05
ATOM	502	OH	TYR	A	109	7.837	28.116	38.668	1.00	28.89
ATOM	503	N	ARG	A	110	12.540	24.995	34.370	1.00	17.31
ATOM	504	CA	ARG	A	110	11.619	24.594	33.311	1.00	17.38
ATOM	505	C	ARG	A	110	11.421	23.077	33.279	1.00	14.31
ATOM	506	O	ARG	A	110	10.316	22.554	33.158	1.00	12.85
ATOM	507	CB	ARG	A	110	12.198	25.061	31.983	1.00	19.68
ATOM	508	CG	ARG	A	110	11.223	24.875	30.835	1.00	21.51
ATOM	509	CD	ARG	A	110	11.719	25.527	29.547	1.00	21.69
ATOM	510	NE	ARG	A	110	10.778	25.285	28.454	1.00	23.64
ATOM	511	CZ	ARG	A	110	10.989	24.203	27.694	1.00	25.84
ATOM	512	NH1	ARG	A	110	12.011	23.397	27.947	1.00	26.19
ATOM	513	NH2	ARG	A	110	10.170	23.951	26.677	1.00	29.07
ATOM	514	N	GLU	A	111	12.559	22.353	33.346	1.00	16.41
ATOM	515	CA	GLU	A	111	12.480	20.893	33.407	1.00	17.69
ATOM	516	C	GLU	A	111	11.636	20.428	34.602	1.00	16.80
ATOM	517	O	GLU	A	111	10.875	19.465	34.534	1.00	17.49
ATOM	518	CB	GLU	A	111	13.908	20.330	33.531	1.00	20.48
ATOM	519	CG	GLU	A	111	14.890	20.946	32.527	1.00	22.16
ATOM	520	CD	GLU	A	111	14.926	20.113	31.254	1.00	22.88
ATOM	521	OE1	GLU	A	111	15.010	18.896	31.346	1.00	27.95
ATOM	522	OE2	GLU	A	111	14.874	20.702	30.170	1.00	22.77
ATOM	523	N	LEU	A	112	11.830	21.132	35.742	1.00	19.48
ATOM	524	CA	LEU	A	112	11.076	20.784	36.943	1.00	17.81
ATOM	525	C	LEU	A	112	9.566	20.847	36.697	1.00	16.62
ATOM	526	O	LEU	A	112	8.833	19.883	36.882	1.00	19.18
ATOM	527	CB	LEU	A	112	11.467	21.774	38.053	1.00	21.80
ATOM	528	CG	LEU	A	112	12.519	21.208	39.020	1.00	22.71

FIG. 2J

ATOM	529	CD1	LEU	A	112	11.898	20.357	40.131	1.00	25.56
ATOM	530	CD2	LEU	A	112	13.549	20.323	38.326	1.00	21.91
ATOM	531	N	VAL	A	113	9.097	22.047	36.280	1.00	20.17
ATOM	532	CA	VAL	A	113	7.651	22.287	36.184	1.00	20.67
ATOM	533	C	VAL	A	113	7.012	21.573	34.990	1.00	20.99
ATOM	534	O	VAL	A	113	5.802	21.406	34.909	1.00	21.37
ATOM	535	CB	VAL	A	113	7.417	23.792	36.067	1.00	22.41
ATOM	536	CG1	VAL	A	113	7.918	24.497	37.324	1.00	25.86
ATOM	537	CG2	VAL	A	113	8.155	24.340	34.857	1.00	27.52
ATOM	538	N	LEU	A	114	7.823	21.155	34.025	1.00	21.23
ATOM	539	CA	LEU	A	114	7.302	20.468	32.852	1.00	23.13
ATOM	540	C	LEU	A	114	6.944	19.040	33.187	1.00	22.69
ATOM	541	O	LEU	A	114	5.970	18.517	32.679	1.00	25.58
ATOM	542	CB	LEU	A	114	8.309	20.510	31.707	1.00	20.01
ATOM	543	CG	LEU	A	114	8.123	21.779	30.910	1.00	16.34
ATOM	544	CD1	LEU	A	114	9.019	21.785	29.697	1.00	16.53
ATOM	545	CD2	LEU	A	114	6.658	21.846	30.529	1.00	20.85
ATOM	546	N	MET	A	115	7.687	18.454	34.114	1.00	26.23
ATOM	547	CA	MET	A	115	7.454	17.093	34.540	1.00	26.25
ATOM	548	C	MET	A	115	6.331	16.986	35.580	1.00	29.91
ATOM	549	O	MET	A	115	6.521	16.426	36.655	1.00	31.74
ATOM	550	CB	MET	A	115	8.745	16.503	35.082	1.00	25.69
ATOM	551	CG	MET	A	115	9.885	16.626	34.109	1.00	25.24
ATOM	552	SD	MET	A	115	11.294	15.590	34.512	1.00	26.61
ATOM	553	CE	MET	A	115	12.674	16.742	34.691	1.00	24.00
ATOM	554	N	LYS	A	116	5.207	17.627	35.295	1.00	28.61
ATOM	555	CA	LYS	A	116	4.016	17.560	36.128	1.00	30.99
ATOM	556	C	LYS	A	116	2.825	17.626	35.157	1.00	33.26
ATOM	557	O	LYS	A	116	1.662	17.676	35.566	1.00	33.76
ATOM	558	CB	LYS	A	116	3.947	18.731	37.115	1.00	33.30
ATOM	559	CG	LYS	A	116	4.682	18.522	38.427	1.00	33.99
ATOM	560	CD	LYS	A	116	6.146	18.859	38.298	1.00	39.13
ATOM	561	CE	LYS	A	116	6.956	18.386	39.509	1.00	42.12
ATOM	562	NZ	LYS	A	116	6.576	19.050	40.806	1.00	42.79
ATOM	563	N	CYS	A	117	3.137	17.548	33.865	1.00	35.37
ATOM	564	CA	CYS	A	117	2.141	17.640	32.801	1.00	39.11
ATOM	565	C	CYS	A	117	2.464	16.718	31.628	1.00	38.05
ATOM	566	O	CYS	A	117	1.953	16.893	30.509	1.00	38.49
ATOM	567	CB	CYS	A	117	2.122	19.070	32.300	1.00	40.82
ATOM	568	SG	CYS	A	117	3.811	19.677	32.161	1.00	52.18
ATOM	569	N	VAL	A	118	3.357	15.772	31.877	1.00	33.83
ATOM	570	CA	VAL	A	118	3.745	14.819	30.869	1.00	29.05
ATOM	571	C	VAL	A	118	3.762	13.424	31.467	1.00	29.19
ATOM	572	O	VAL	A	118	4.564	13.130	32.350	1.00	32.10
ATOM	573	CB	VAL	A	118	5.115	15.167	30.286	1.00	22.96
ATOM	574	CG1	VAL	A	118	5.005	16.461	29.515	1.00	23.45
ATOM	575	CG2	VAL	A	118	6.169	15.270	31.382	1.00	21.58
ATOM	576	N	THR	A	119	2.805	12.594	31.071	1.00	28.43
ATOM	577	CA	THR	A	119	2.773	11.232	31.580	1.00	26.35
ATOM	578	C	THR	A	119	2.964	10.272	30.401	1.00	21.80
ATOM	579	O	THR	A	119	2.026	9.812	29.759	1.00	17.32
ATOM	580	CB	THR	A	119	1.499	10.962	32.474	1.00	29.38
ATOM	581	OG1	THR	A	119	1.657	9.720	33.177	1.00	28.88
ATOM	582	CG2	THR	A	119	0.187	10.966	31.656	1.00	28.91
ATOM	583	N	HIS	A	120	4.229	10.043	30.077	1.00	21.71
ATOM	584	CA	HIS	A	120	4.538	9.181	28.971	1.00	18.80
ATOM	585	C	HIS	A	120	5.749	8.329	29.189	1.00	19.60
ATOM	586	O	HIS	A	120	6.767	8.795	29.673	1.00	18.49
ATOM	587	CB	HIS	A	120	4.714	9.979	27.697	1.00	22.81

FIG. 2K

ATOM	588	CG	HIS	A	120	4.446	9.182	26.457	1.00	19.79
ATOM	589	ND1	HIS	A	120	3.174	8.948	25.993	1.00	20.77
ATOM	590	CD2	HIS	A	120	5.285	8.571	25.595	1.00	21.10
ATOM	591	CE1	HIS	A	120	3.236	8.229	24.887	1.00	20.93
ATOM	592	NE2	HIS	A	120	4.507	7.984	24.623	1.00	22.50
ATOM	593	N	LYS	A	121	5.632	7.093	28.702	1.00	21.55
ATOM	594	CA	LYS	A	121	6.652	6.069	28.798	1.00	18.22
ATOM	595	C	LYS	A	121	7.858	6.406	27.956	1.00	15.50
ATOM	596	O	LYS	A	121	8.958	5.894	28.204	1.00	13.13
ATOM	597	CB	LYS	A	121	6.061	4.700	28.425	1.00	23.17
ATOM	598	CG	LYS	A	121	5.211	4.668	27.137	1.00	24.31
ATOM	599	CD	LYS	A	121	4.637	3.295	26.862	1.00	23.40
ATOM	600	CE	LYS	A	121	5.738	2.249	26.709	1.00	27.84
ATOM	601	NZ	LYS	A	121	5.208	0.856	26.420	1.00	31.61
ATOM	602	N	ASN	A	122	7.662	7.328	27.008	1.00	17.11
ATOM	603	CA	ASN	A	122	8.741	7.778	26.123	1.00	17.46
ATOM	604	C	ASN	A	122	9.369	9.120	26.527	1.00	17.20
ATOM	605	O	ASN	A	122	10.325	9.589	25.898	1.00	16.39
ATOM	606	CB	ASN	A	122	8.255	7.788	24.675	1.00	15.86
ATOM	607	CG	ASN	A	122	7.777	6.435	24.232	1.00	12.87
ATOM	608	OD1	ASN	A	122	6.661	6.282	23.774	1.00	11.71
ATOM	609	ND2	ASN	A	122	8.609	5.430	24.435	1.00	11.51
ATOM	610	N	ILE	A	123	8.835	9.717	27.590	1.00	18.46
ATOM	611	CA	ILE	A	123	9.346	10.980	28.131	1.00	20.03
ATOM	612	C	ILE	A	123	9.827	10.696	29.557	1.00	19.81
ATOM	613	O	ILE	A	123	9.234	9.878	30.269	1.00	19.83
ATOM	614	CB	ILE	A	123	8.274	12.111	28.216	1.00	16.40
ATOM	615	CG1	ILE	A	123	7.667	12.431	26.837	1.00	18.54
ATOM	616	CG2	ILE	A	123	8.889	13.316	28.880	1.00	14.23
ATOM	617	CD1	ILE	A	123	8.676	12.778	25.747	1.00	14.50
ATOM	618	N	ILE	A	124	10.885	11.382	29.982	1.00	21.80
ATOM	619	CA	ILE	A	124	11.444	11.194	31.320	1.00	21.44
ATOM	620	C	ILE	A	124	10.435	11.441	32.440	1.00	20.65
ATOM	621	O	ILE	A	124	9.611	12.360	32.384	1.00	17.78
ATOM	622	CB	ILE	A	124	12.681	12.089	31.552	1.00	23.19
ATOM	623	CG1	ILE	A	124	13.191	11.918	32.985	1.00	21.54
ATOM	624	CG2	ILE	A	124	12.343	13.531	31.233	1.00	22.16
ATOM	625	CD1	ILE	A	124	14.248	12.902	33.409	1.00	25.57
ATOM	626	N	SER	A	125	10.479	10.549	33.428	1.00	25.24
ATOM	627	CA	SER	A	125	9.622	10.584	34.629	1.00	25.57
ATOM	628	C	SER	A	125	10.533	10.584	35.852	1.00	22.29
ATOM	629	O	SER	A	125	11.474	9.799	35.943	1.00	19.83
ATOM	630	CB	SER	A	125	8.734	9.328	34.726	1.00	29.09
ATOM	631	OG	SER	A	125	7.709	9.260	33.751	1.00	39.45
ATOM	632	N	LEU	A	126	10.225	11.425	36.819	1.00	21.25
ATOM	633	CA	LEU	A	126	11.059	11.458	37.995	1.00	21.80
ATOM	634	C	LEU	A	126	10.529	10.576	39.140	1.00	20.60
ATOM	635	O	LEU	A	126	9.315	10.470	39.376	1.00	15.37
ATOM	636	CB	LEU	A	126	11.276	12.907	38.418	1.00	26.09
ATOM	637	CG	LEU	A	126	12.013	13.745	37.363	1.00	24.09
ATOM	638	CD1	LEU	A	126	12.074	15.165	37.840	1.00	27.50
ATOM	639	CD2	LEU	A	126	13.421	13.246	37.149	1.00	21.86
ATOM	640	N	LEU	A	127	11.449	9.843	39.759	1.00	19.81
ATOM	641	CA	LEU	A	127	11.119	8.960	40.878	1.00	16.92
ATOM	642	C	LEU	A	127	11.264	9.740	42.183	1.00	17.28
ATOM	643	O	LEU	A	127	10.511	9.525	43.135	1.00	18.90
ATOM	644	CB	LEU	A	127	12.098	7.793	40.924	1.00	11.43
ATOM	645	CG	LEU	A	127	11.998	6.826	39.769	1.00	7.89
ATOM	646	CD1	LEU	A	127	13.068	5.751	39.875	1.00	4.22

FIG. 2L

ATOM	647	CD2	LEU	A	127	10.606	6.278	39.816	1.00	8.16
ATOM	648	N	ASN	A	128	12.231	10.654	42.192	1.00	16.69
ATOM	649	CA	ASN	A	128	12.539	11.446	43.353	1.00	18.74
ATOM	650	C	ASN	A	128	13.351	12.676	42.968	1.00	18.70
ATOM	651	O	ASN	A	128	14.103	12.660	41.991	1.00	18.08
ATOM	652	CB	ASN	A	128	13.353	10.584	44.330	1.00	19.51
ATOM	653	CG	ASN	A	128	13.348	11.125	45.753	1.00	17.80
ATOM	654	OD1	ASN	A	128	14.249	10.836	46.542	1.00	17.49
ATOM	655	ND2	ASN	A	128	12.307	11.863	46.100	1.00	12.82
ATOM	656	N	VAL	A	129	13.135	13.748	43.732	1.00	19.15
ATOM	657	CA	VAL	A	129	13.838	15.033	43.600	1.00	18.43
ATOM	658	C	VAL	A	129	14.154	15.415	45.038	1.00	14.75
ATOM	659	O	VAL	A	129	13.290	15.335	45.902	1.00	16.11
ATOM	660	CB	VAL	A	129	12.923	16.178	43.039	1.00	17.78
ATOM	661	CG1	VAL	A	129	13.751	17.457	42.790	1.00	17.05
ATOM	662	CG2	VAL	A	129	12.207	15.726	41.790	1.00	17.58
ATOM	663	N	PHE	A	130	15.367	15.830	45.321	1.00	12.66
ATOM	664	CA	PHE	A	130	15.631	16.194	46.680	1.00	14.68
ATOM	665	C	PHE	A	130	16.845	17.095	46.773	1.00	14.31
ATOM	666	O	PHE	A	130	17.567	17.283	45.802	1.00	14.60
ATOM	667	CB	PHE	A	130	15.835	14.914	47.533	1.00	11.21
ATOM	668	CG	PHE	A	130	17.098	14.147	47.199	1.00	6.13
ATOM	669	CD1	PHE	A	130	17.060	13.050	46.351	1.00	5.37
ATOM	670	CD2	PHE	A	130	18.311	14.555	47.690	1.00	2.00
ATOM	671	CE1	PHE	A	130	18.212	12.387	46.016	1.00	2.00
ATOM	672	CE2	PHE	A	130	19.468	13.894	47.358	1.00	2.88
ATOM	673	CZ	PHE	A	130	19.409	12.807	46.506	1.00	2.00
ATOM	674	N	THR	A	131	17.019	17.705	47.940	1.00	14.01
ATOM	675	CA	THR	A	131	18.182	18.530	48.197	1.00	9.41
ATOM	676	C	THR	A	131	18.618	18.323	49.616	1.00	8.55
ATOM	677	O	THR	A	131	17.817	18.310	50.526	1.00	8.61
ATOM	678	CB	THR	A	131	17.948	20.064	47.962	1.00	11.54
ATOM	679	OG1	THR	A	131	19.126	20.772	48.335	1.00	8.08
ATOM	680	CG2	THR	A	131	16.781	20.604	48.770	1.00	5.13
ATOM	681	N	PRO	A	132	19.902	18.071	49.806	1.00	10.38
ATOM	682	CA	PRO	A	132	20.434	17.872	51.149	1.00	13.25
ATOM	683	C	PRO	A	132	20.595	19.173	51.959	1.00	17.66
ATOM	684	O	PRO	A	132	21.428	19.233	52.856	1.00	21.50
ATOM	685	CB	PRO	A	132	21.798	17.237	50.865	1.00	11.28
ATOM	686	CG	PRO	A	132	22.169	17.744	49.510	1.00	7.43
ATOM	687	CD	PRO	A	132	20.873	17.659	48.785	1.00	8.12
ATOM	688	N	GLN	A	133	19.841	20.223	51.642	1.00	17.79
ATOM	689	CA	GLN	A	133	19.971	21.483	52.373	1.00	14.40
ATOM	690	C	GLN	A	133	18.638	21.805	52.969	1.00	15.53
ATOM	691	O	GLN	A	133	17.619	21.718	52.292	1.00	15.63
ATOM	692	CB	GLN	A	133	20.452	22.599	51.460	1.00	15.11
ATOM	693	CG	GLN	A	133	21.948	22.515	51.141	1.00	7.56
ATOM	694	CD	GLN	A	133	22.230	21.958	49.781	1.00	6.70
ATOM	695	OE1	GLN	A	133	23.330	21.479	49.511	1.00	5.45
ATOM	696	NE2	GLN	A	133	21.243	22.024	48.901	1.00	6.69
ATOM	697	N	LYS	A	134	18.638	22.169	54.249	1.00	21.20
ATOM	698	CA	LYS	A	134	17.385	22.410	54.949	1.00	23.36
ATOM	699	C	LYS	A	134	16.695	23.726	54.799	1.00	23.18
ATOM	700	O	LYS	A	134	15.473	23.792	54.976	1.00	23.37
ATOM	701	CB	LYS	A	134	17.472	22.008	56.440	1.00	25.32
ATOM	702	CG	LYS	A	134	18.752	22.374	57.183	1.00	33.07
ATOM	703	CD	LYS	A	134	18.695	21.936	58.677	1.00	37.91
ATOM	704	CE	LYS	A	134	19.020	20.435	58.888	1.00	39.95
ATOM	705	NZ	LYS	A	134	18.837	19.935	60.304	1.00	40.52

FIG. 2M

ATOM	706	N	THR	A	135	17.456	24.767	54.465	1.00	24.81
ATOM	707	CA	THR	A	135	16.879	26.101	54.311	1.00	22.85
ATOM	708	C	THR	A	135	17.225	26.694	52.975	1.00	22.80
ATOM	709	O	THR	A	135	18.295	26.415	52.431	1.00	21.61
ATOM	710	CB	THR	A	135	17.400	27.095	55.377	1.00	23.37
ATOM	711	OG1	THR	A	135	18.801	27.324	55.165	1.00	21.29
ATOM	712	CG2	THR	A	135	17.145	26.561	56.816	1.00	23.04
ATOM	713	N	LEU	A	136	16.357	27.590	52.506	1.00	23.87
ATOM	714	CA	LEU	A	136	16.553	28.277	51.240	1.00	24.40
ATOM	715	C	LEU	A	136	17.903	28.973	51.250	1.00	26.61
ATOM	716	O	LEU	A	136	18.569	29.073	50.221	1.00	30.85
ATOM	717	CB	LEU	A	136	15.436	29.283	51.002	1.00	25.03
ATOM	718	CG	LEU	A	136	15.414	29.920	49.606	1.00	24.06
ATOM	719	CD1	LEU	A	136	13.978	30.253	49.226	1.00	24.03
ATOM	720	CD2	LEU	A	136	16.306	31.150	49.576	1.00	17.83
ATOM	721	N	GLU	A	137	18.337	29.408	52.426	1.00	25.92
ATOM	722	CA	GLU	A	137	19.624	30.068	52.515	1.00	25.21
ATOM	723	C	GLU	A	137	20.757	29.089	52.378	1.00	22.62
ATOM	724	O	GLU	A	137	21.843	29.476	51.969	1.00	24.90
ATOM	725	CB	GLU	A	137	19.788	30.843	53.826	1.00	29.36
ATOM	726	CG	GLU	A	137	18.953	32.090	53.899	1.00	30.88
ATOM	727	CD	GLU	A	137	17.496	31.780	54.062	1.00	33.67
ATOM	728	OE1	GLU	A	137	17.137	31.250	55.138	1.00	36.89
ATOM	729	OE2	GLU	A	137	16.709	32.072	53.129	1.00	37.00
ATOM	730	N	GLU	A	138	20.546	27.837	52.770	1.00	23.41
ATOM	731	CA	GLU	A	138	21.625	26.842	52.645	1.00	23.74
ATOM	732	C	GLU	A	138	21.701	26.229	51.261	1.00	20.15
ATOM	733	O	GLU	A	138	22.770	25.803	50.825	1.00	15.33
ATOM	734	CB	GLU	A	138	21.480	25.743	53.693	1.00	28.37
ATOM	735	CG	GLU	A	138	21.658	26.257	55.099	1.00	34.15
ATOM	736	CD	GLU	A	138	21.176	25.270	56.135	1.00	39.34
ATOM	737	OE1	GLU	A	138	19.942	25.123	56.308	1.00	41.01
ATOM	738	OE2	GLU	A	138	22.037	24.648	56.791	1.00	44.64
ATOM	739	N	PHE	A	139	20.562	26.265	50.574	1.00	20.75
ATOM	740	CA	PHE	A	139	20.368	25.716	49.234	1.00	22.38
ATOM	741	C	PHE	A	139	21.476	25.906	48.215	1.00	22.59
ATOM	742	O	PHE	A	139	21.907	27.019	47.942	1.00	22.05
ATOM	743	CB	PHE	A	139	19.085	26.253	48.630	1.00	22.29
ATOM	744	CG	PHE	A	139	18.688	25.559	47.353	1.00	26.18
ATOM	745	CD1	PHE	A	139	18.798	24.177	47.242	1.00	27.65
ATOM	746	CD2	PHE	A	139	18.183	26.275	46.276	1.00	27.40
ATOM	747	CE1	PHE	A	139	18.412	23.520	46.083	1.00	26.62
ATOM	748	CE2	PHE	A	139	17.788	25.623	45.097	1.00	27.97
ATOM	749	CZ	PHE	A	139	17.904	24.250	45.003	1.00	24.56
ATOM	750	N	GLN	A	140	21.942	24.790	47.664	1.00	23.18
ATOM	751	CA	GLN	A	140	22.980	24.792	46.648	1.00	20.44
ATOM	752	C	GLN	A	140	22.660	23.838	45.507	1.00	19.37
ATOM	753	O	GLN	A	140	22.604	24.250	44.343	1.00	18.41
ATOM	754	CB	GLN	A	140	24.330	24.427	47.254	1.00	15.98
ATOM	755	CG	GLN	A	140	24.911	25.536	48.072	1.00	23.25
ATOM	756	CD	GLN	A	140	26.398	25.358	48.285	1.00	30.69
ATOM	757	OE1	GLN	A	140	26.836	24.443	48.994	1.00	35.70
ATOM	758	NE2	GLN	A	140	27.192	26.249	47.696	1.00	35.47
ATOM	759	N	ASP	A	141	22.390	22.578	45.871	1.00	20.11
ATOM	760	CA	ASP	A	141	22.122	21.511	44.911	1.00	14.85
ATOM	761	C	ASP	A	141	20.763	20.809	44.853	1.00	11.85
ATOM	762	O	ASP	A	141	20.069	20.634	45.851	1.00	12.51
ATOM	763	CB	ASP	A	141	23.227	20.490	45.044	1.00	13.73
ATOM	764	CG	ASP	A	141	24.583	21.127	45.096	1.00	13.36

FIG. 2N

ATOM	765	OD1	ASP	A	141	25.429	20.722	45.911	1.00	17.82
ATOM	766	OD2	ASP	A	141	24.820	22.072	44.340	1.00	18.36
ATOM	767	N	VAL	A	142	20.394	20.421	43.638	1.00	14.47
ATOM	768	CA	VAL	A	142	19.157	19.705	43.324	1.00	12.88
ATOM	769	C	VAL	A	142	19.522	18.335	42.744	1.00	13.98
ATOM	770	O	VAL	A	142	20.330	18.222	41.807	1.00	13.92
ATOM	771	CB	VAL	A	142	18.319	20.492	42.321	1.00	15.25
ATOM	772	CG1	VAL	A	142	17.143	19.650	41.822	1.00	8.68
ATOM	773	CG2	VAL	A	142	17.858	21.802	42.988	1.00	13.03
ATOM	774	N	TYR	A	143	18.957	17.285	43.339	1.00	13.49
ATOM	775	CA	TYR	A	143	19.254	15.907	42.929	1.00	10.05
ATOM	776	C	TYR	A	143	18.036	15.312	42.298	1.00	8.26
ATOM	777	O	TYR	A	143	16.963	15.333	42.875	1.00	8.82
ATOM	778	CB	TYR	A	143	19.726	15.043	44.119	1.00	5.83
ATOM	779	CG	TYR	A	143	21.153	15.323	44.558	1.00	2.00
ATOM	780	CD1	TYR	A	143	21.445	16.389	45.400	1.00	3.10
ATOM	781	CD2	TYR	A	143	22.202	14.537	44.139	1.00	2.00
ATOM	782	CE1	TYR	A	143	22.709	16.647	45.794	1.00	2.00
ATOM	783	CE2	TYR	A	143	23.495	14.799	44.546	1.00	2.00
ATOM	784	CZ	TYR	A	143	23.732	15.869	45.382	1.00	2.00
ATOM	785	OH	TYR	A	143	25.011	16.177	45.802	1.00	5.05
ATOM	786	N	LEU	A	144	18.202	14.841	41.069	1.00	12.03
ATOM	787	CA	LEU	A	144	17.091	14.260	40.328	1.00	12.86
ATOM	788	C	LEU	A	144	17.301	12.773	40.197	1.00	9.40
ATOM	789	O	LEU	A	144	18.434	12.304	40.029	1.00	10.24
ATOM	790	CB	LEU	A	144	16.960	14.915	38.936	1.00	12.95
ATOM	791	CG	LEU	A	144	16.637	16.413	38.922	1.00	14.49
ATOM	792	CD1	LEU	A	144	17.061	16.992	37.585	1.00	15.65
ATOM	793	CD2	LEU	A	144	15.152	16.691	39.211	1.00	10.66
ATOM	794	N	VAL	A	145	16.201	12.033	40.273	1.00	9.00
ATOM	795	CA	VAL	A	145	16.275	10.587	40.177	1.00	7.36
ATOM	796	C	VAL	A	145	15.288	10.023	39.164	1.00	2.00
ATOM	797	O	VAL	A	145	14.155	10.461	39.112	1.00	2.00
ATOM	798	CB	VAL	A	145	16.010	9.942	41.578	1.00	8.11
ATOM	799	CG1	VAL	A	145	15.928	8.459	41.449	1.00	6.36
ATOM	800	CG2	VAL	A	145	17.131	10.268	42.535	1.00	10.32
ATOM	801	N	MET	A	146	15.740	9.060	38.360	1.00	6.09
ATOM	802	CA	MET	A	146	14.891	8.380	37.351	1.00	11.90
ATOM	803	C	MET	A	146	15.283	6.891	37.270	1.00	12.67
ATOM	804	O	MET	A	146	16.385	6.533	37.681	1.00	16.93
ATOM	805	CB	MET	A	146	15.112	8.995	35.958	1.00	13.21
ATOM	806	CG	MET	A	146	16.477	8.650	35.322	1.00	14.34
ATOM	807	SD	MET	A	146	16.595	9.005	33.507	1.00	17.24
ATOM	808	CE	MET	A	146	15.195	8.091	32.828	1.00	8.30
ATOM	809	N	GLU	A	147	14.427	6.027	36.720	1.00	13.63
ATOM	810	CA	GLU	A	147	14.795	4.614	36.616	1.00	16.06
ATOM	811	C	GLU	A	147	16.041	4.564	35.742	1.00	16.39
ATOM	812	O	GLU	A	147	16.138	5.299	34.772	1.00	18.15
ATOM	813	CB	GLU	A	147	13.660	3.769	36.015	1.00	22.30
ATOM	814	CG	GLU	A	147	13.269	4.118	34.575	1.00	25.11
ATOM	815	CD	GLU	A	147	12.876	2.894	33.729	1.00	25.31
ATOM	816	OE1	GLU	A	147	13.782	2.106	33.394	1.00	30.02
ATOM	817	OE2	GLU	A	147	11.686	2.723	33.368	1.00	23.23
ATOM	818	N	LEU	A	148	17.013	3.733	36.096	1.00	14.22
ATOM	819	CA	LEU	A	148	18.251	3.652	35.343	1.00	14.03
ATOM	820	C	LEU	A	148	18.138	3.001	33.953	1.00	19.58
ATOM	821	O	LEU	A	148	17.489	1.954	33.772	1.00	17.45
ATOM	822	CB	LEU	A	148	19.315	2.944	36.172	1.00	11.14
ATOM	823	CG	LEU	A	148	20.705	2.855	35.560	1.00	11.21

FIG. 20

ATOM	824	CD1	LEU	A	148	21.451	4.189	35.640	1.00	13.69
ATOM	825	CD2	LEU	A	148	21.464	1.797	36.305	1.00	12.65
ATOM	826	N	MET	A	149	18.820	3.619	32.988	1.00	18.65
ATOM	827	CA	MET	A	149	18.820	3.148	31.618	1.00	14.79
ATOM	828	C	MET	A	149	20.130	2.454	31.345	1.00	13.07
ATOM	829	O	MET	A	149	21.072	2.559	32.123	1.00	11.86
ATOM	830	CB	MET	A	149	18.658	4.327	30.640	1.00	14.73
ATOM	831	CG	MET	A	149	17.373	5.086	30.763	1.00	5.61
ATOM	832	SD	MET	A	149	15.962	4.060	30.627	1.00	10.51
ATOM	833	CE	MET	A	149	15.493	4.372	28.976	1.00	9.66
ATOM	834	N	ASP	A	150	20.207	1.802	30.184	1.00	14.05
ATOM	835	CA	ASP	A	150	21.413	1.085	29.787	1.00	11.22
ATOM	836	C	ASP	A	150	22.380	1.845	28.922	1.00	10.09
ATOM	837	O	ASP	A	150	23.575	1.506	28.898	1.00	10.09
ATOM	838	CB	ASP	A	150	21.037	-0.230	29.130	1.00	16.26
ATOM	839	CG	ASP	A	150	20.243	-1.117	30.037	1.00	13.51
ATOM	840	OD1	ASP	A	150	20.675	-1.305	31.189	1.00	21.61
ATOM	841	OD2	ASP	A	150	19.177	-1.594	29.635	1.00	14.13
ATOM	842	N	ALA	A	151	21.892	2.860	28.203	1.00	12.49
ATOM	843	CA	ALA	A	151	22.895	3.532	27.362	1.00	11.41
ATOM	844	C	ALA	A	151	22.325	4.780	26.650	1.00	6.60
ATOM	845	O	ALA	A	151	21.144	5.071	26.685	1.00	9.62
ATOM	846	CB	ALA	A	151	23.395	2.525	26.321	1.00	15.41
ATOM	847	N	ASN	A	152	23.255	5.559	26.017	1.00	8.84
ATOM	848	CA	ASN	A	152	22.834	6.768	25.269	1.00	12.68
ATOM	849	C	ASN	A	152	22.463	6.411	23.827	1.00	14.17
ATOM	850	O	ASN	A	152	22.850	5.384	23.299	1.00	12.97
ATOM	851	CB	ASN	A	152	24.018	7.753	25.259	1.00	15.88
ATOM	852	CG	ASN	A	152	23.540	9.137	25.583	1.00	21.57
ATOM	853	OD1	ASN	A	152	22.347	9.428	25.598	1.00	22.60
ATOM	854	ND2	ASN	A	152	24.517	10.021	25.847	1.00	22.95
ATOM	855	N	LEU	A	153	21.664	7.294	23.186	1.00	15.15
ATOM	856	CA	LEU	A	153	21.356	7.079	21.769	1.00	15.28
ATOM	857	C	LEU	A	153	22.606	7.253	20.909	1.00	17.68
ATOM	858	O	LEU	A	153	22.734	6.709	19.820	1.00	21.55
ATOM	859	CB	LEU	A	153	20.278	8.089	21.339	1.00	15.66
ATOM	860	CG	LEU	A	153	19.170	7.451	20.478	1.00	17.15
ATOM	861	CD1	LEU	A	153	18.727	8.359	19.327	1.00	10.86
ATOM	862	CD2	LEU	A	153	19.602	6.127	19.840	1.00	16.75
ATOM	863	N	CYS	A	154	23.616	7.963	21.398	1.00	20.01
ATOM	864	CA	CYS	A	154	24.877	8.139	20.688	1.00	21.31
ATOM	865	C	CYS	A	154	25.586	6.786	20.532	1.00	24.69
ATOM	866	O	CYS	A	154	26.235	6.509	19.517	1.00	23.42
ATOM	867	CB	CYS	A	154	25.806	9.047	21.498	1.00	21.53
ATOM	868	SG	CYS	A	154	25.188	10.670	21.924	1.00	19.73
ATOM	869	N	ALA	A	155	25.515	5.985	21.587	1.00	24.09
ATOM	870	CA	ALA	A	155	26.140	4.682	21.615	1.00	22.22
ATOM	871	C	ALA	A	155	25.415	3.715	20.676	1.00	21.75
ATOM	872	O	ALA	A	155	26.062	2.949	19.958	1.00	20.49
ATOM	873	CB	ALA	A	155	26.139	4.153	23.053	1.00	22.67
ATOM	874	N	VAL	A	156	24.081	3.791	20.654	1.00	20.79
ATOM	875	CA	VAL	A	156	23.256	2.936	19.800	1.00	19.64
ATOM	876	C	VAL	A	156	23.401	3.318	18.324	1.00	21.10
ATOM	877	O	VAL	A	156	23.276	2.463	17.456	1.00	22.67
ATOM	878	CB	VAL	A	156	21.757	3.013	20.202	1.00	18.09
ATOM	879	CG1	VAL	A	156	20.898	2.256	19.209	1.00	18.46
ATOM	880	CG2	VAL	A	156	21.552	2.450	21.586	1.00	18.31
ATOM	881	N	ILE	A	157	23.665	4.597	18.046	1.00	21.10
ATOM	882	CA	ILE	A	157	23.832	5.101	16.681	1.00	21.62

FIG. 2P

ATOM	883	C	ILE	A	157	25.082	4.471	16.108	1.00	21.87
ATOM	884	O	ILE	A	157	25.191	4.226	14.898	1.00	20.25
ATOM	885	CB	ILE	A	157	24.016	6.669	16.641	1.00	21.74
ATOM	886	CG1	ILE	A	157	22.662	7.363	16.670	1.00	20.08
ATOM	887	CG2	ILE	A	157	24.737	7.106	15.372	1.00	22.36
ATOM	888	CD1	ILE	A	157	22.762	8.840	16.733	1.00	21.43
ATOM	889	N	GLN	A	158	26.031	4.228	16.998	1.00	20.23
ATOM	890	CA	GLN	A	158	27.278	3.643	16.622	1.00	19.49
ATOM	891	C	GLN	A	158	27.186	2.171	16.296	1.00	21.66
ATOM	892	O	GLN	A	158	28.176	1.580	15.856	1.00	24.62
ATOM	893	CB	GLN	A	158	28.276	3.816	17.732	1.00	22.75
ATOM	894	CG	GLN	A	158	28.931	5.157	17.809	1.00	25.62
ATOM	895	CD	GLN	A	158	30.303	5.003	18.384	1.00	28.38
ATOM	896	OE1	GLN	A	158	31.220	4.555	17.687	1.00	29.99
ATOM	897	NE2	GLN	A	158	30.449	5.292	19.677	1.00	29.10
ATOM	898	N	MET	A	159	26.054	1.540	16.571	1.00	19.31
ATOM	899	CA	MET	A	159	25.972	0.139	16.250	1.00	19.50
ATOM	900	C	MET	A	159	25.159	-0.138	15.011	1.00	23.14
ATOM	901	O	MET	A	159	24.439	0.720	14.505	1.00	24.42
ATOM	902	CB	MET	A	159	25.515	-0.695	17.439	1.00	15.90
ATOM	903	CG	MET	A	159	24.179	-0.404	17.999	1.00	14.14
ATOM	904	SD	MET	A	159	24.233	-0.841	19.784	1.00	23.46
ATOM	905	CE	MET	A	159	22.592	-1.324	19.992	1.00	14.23
ATOM	906	N	GLU	A	160	25.355	-1.325	14.469	1.00	24.45
ATOM	907	CA	GLU	A	160	24.657	-1.738	13.283	1.00	25.01
ATOM	908	C	GLU	A	160	23.360	-2.398	13.709	1.00	28.90
ATOM	909	O	GLU	A	160	23.375	-3.495	14.260	1.00	32.36
ATOM	910	CB	GLU	A	160	25.531	-2.727	12.536	1.00	23.25
ATOM	911	CG	GLU	A	160	25.228	-2.838	11.093	1.00	27.17
ATOM	912	CD	GLU	A	160	26.211	-3.734	10.392	1.00	26.17
ATOM	913	OE1	GLU	A	160	26.054	-4.957	10.529	1.00	27.98
ATOM	914	OE2	GLU	A	160	27.143	-3.226	9.725	1.00	31.36
ATOM	915	N	LEU	A	161	22.240	-1.701	13.551	1.00	29.29
ATOM	916	CA	LEU	A	161	20.970	-2.295	13.937	1.00	29.26
ATOM	917	C	LEU	A	161	20.017	-2.532	12.780	1.00	28.20
ATOM	918	O	LEU	A	161	20.024	-1.820	11.769	1.00	29.99
ATOM	919	CB	LEU	A	161	20.270	-1.519	15.066	1.00	31.73
ATOM	920	CG	LEU	A	161	19.907	-0.042	15.005	1.00	30.31
ATOM	921	CD1	LEU	A	161	19.055	0.288	16.210	1.00	29.64
ATOM	922	CD2	LEU	A	161	21.170	0.803	15.010	1.00	35.08
ATOM	923	N	ASP	A	162	19.212	-3.566	12.948	1.00	24.93
ATOM	924	CA	ASP	A	162	18.233	-3.967	11.968	1.00	23.67
ATOM	925	C	ASP	A	162	17.157	-2.910	11.812	1.00	21.63
ATOM	926	O	ASP	A	162	17.296	-1.815	12.315	1.00	24.12
ATOM	927	CB	ASP	A	162	17.622	-5.284	12.401	1.00	21.90
ATOM	928	CG	ASP	A	162	17.261	-5.276	13.848	1.00	20.75
ATOM	929	OD1	ASP	A	162	16.067	-5.078	14.151	1.00	24.78
ATOM	930	OD2	ASP	A	162	18.175	-5.442	14.680	1.00	23.53
ATOM	931	N	HIS	A	163	16.106	-3.247	11.070	1.00	23.69
ATOM	932	CA	HIS	A	163	14.984	-2.340	10.815	1.00	24.26
ATOM	933	C	HIS	A	163	13.937	-2.378	11.898	1.00	24.23
ATOM	934	O	HIS	A	163	13.153	-1.435	12.051	1.00	25.59
ATOM	935	CB	HIS	A	163	14.324	-2.664	9.454	1.00	25.62
ATOM	936	CG	HIS	A	163	15.174	-2.305	8.272	1.00	27.11
ATOM	937	ND1	HIS	A	163	15.328	-1.005	7.831	1.00	24.70
ATOM	938	CD2	HIS	A	163	15.945	-3.070	7.462	1.00	28.10
ATOM	939	CE1	HIS	A	163	16.157	-0.987	6.804	1.00	24.28
ATOM	940	NE2	HIS	A	163	16.546	-2.226	6.559	1.00	26.23
ATOM	941	N	GLU	A	164	13.915	-3.474	12.649	1.00	25.49

FIG. 2Q

ATOM	942	CA	GLU	A	164	12.936	-3.650	13.720	1.00	23.13
ATOM	943	C	GLU	A	164	13.295	-2.753	14.904	1.00	15.55
ATOM	944	O	GLU	A	164	12.427	-2.141	15.513	1.00	14.60
ATOM	945	CB	GLU	A	164	12.883	-5.124	14.129	1.00	29.26
ATOM	946	CG	GLU	A	164	12.827	-6.092	12.934	1.00	37.97
ATOM	947	CD	GLU	A	164	13.817	-7.263	13.074	1.00	43.81
ATOM	948	OE1	GLU	A	164	14.826	-7.294	12.326	1.00	45.99
ATOM	949	OE2	GLU	A	164	13.589	-8.150	13.935	1.00	44.01
ATOM	950	N	ARG	A	165	14.584	-2.672	15.189	1.00	12.40
ATOM	951	CA	ARG	A	165	15.110	-1.846	16.261	1.00	15.54
ATOM	952	C	ARG	A	165	15.050	-0.355	15.857	1.00	18.06
ATOM	953	O	ARG	A	165	14.479	0.488	16.556	1.00	17.13
ATOM	954	CB	ARG	A	165	16.563	-2.228	16.498	1.00	14.64
ATOM	955	CG	ARG	A	165	16.793	-3.685	16.735	1.00	18.72
ATOM	956	CD	ARG	A	165	16.848	-4.072	18.198	1.00	21.86
ATOM	957	NE	ARG	A	165	16.861	-5.527	18.362	1.00	26.60
ATOM	958	CZ	ARG	A	165	17.943	-6.293	18.269	1.00	27.31
ATOM	959	NH1	ARG	A	165	19.135	-5.752	18.028	1.00	30.44
ATOM	960	NH2	ARG	A	165	17.820	-7.609	18.351	1.00	27.82
ATOM	961	N	MET	A	166	15.642	-0.066	14.701	1.00	18.91
ATOM	962	CA	MET	A	166	15.702	1.257	14.121	1.00	16.85
ATOM	963	C	MET	A	166	14.330	1.897	14.082	1.00	16.90
ATOM	964	O	MET	A	166	14.147	3.007	14.573	1.00	17.46
ATOM	965	CB	MET	A	166	16.276	1.147	12.716	1.00	21.41
ATOM	966	CG	MET	A	166	16.493	2.449	11.988	1.00	24.12
ATOM	967	SD	MET	A	166	18.115	2.432	11.226	1.00	32.52
ATOM	968	CE	MET	A	166	18.074	0.866	10.278	1.00	32.32
ATOM	969	N	SER	A	167	13.343	1.187	13.559	1.00	14.77
ATOM	970	CA	SER	A	167	11.996	1.716	13.487	1.00	14.86
ATOM	971	C	SER	A	167	11.204	1.763	14.805	1.00	17.43
ATOM	972	O	SER	A	167	10.276	2.576	14.917	1.00	18.84
ATOM	973	CB	SER	A	167	11.195	0.953	12.437	1.00	18.44
ATOM	974	OG	SER	A	167	11.017	-0.404	12.823	1.00	21.45
ATOM	975	N	TYR	A	168	11.483	0.859	15.764	1.00	17.75
ATOM	976	CA	TYR	A	168	10.768	0.868	17.047	1.00	14.06
ATOM	977	C	TYR	A	168	11.286	2.086	17.785	1.00	12.00
ATOM	978	O	TYR	A	168	10.531	2.827	18.400	1.00	12.54
ATOM	979	CB	TYR	A	168	11.026	-0.410	17.879	1.00	14.32
ATOM	980	CG	TYR	A	168	10.261	-0.453	19.200	1.00	10.40
ATOM	981	CD1	TYR	A	168	8.896	-0.211	19.247	1.00	14.66
ATOM	982	CD2	TYR	A	168	10.905	-0.698	20.401	1.00	12.40
ATOM	983	CE1	TYR	A	168	8.196	-0.201	20.467	1.00	14.22
ATOM	984	CE2	TYR	A	168	10.208	-0.697	21.623	1.00	6.91
ATOM	985	CZ	TYR	A	168	8.865	-0.445	21.648	1.00	11.44
ATOM	986	OH	TYR	A	168	8.174	-0.426	22.854	1.00	15.18
ATOM	987	N	LEU	A	169	12.586	2.298	17.686	1.00	10.99
ATOM	988	CA	LEU	A	169	13.221	3.447	18.293	1.00	13.26
ATOM	989	C	LEU	A	169	12.631	4.756	17.748	1.00	15.32
ATOM	990	O	LEU	A	169	12.190	5.621	18.516	1.00	14.97
ATOM	991	CB	LEU	A	169	14.719	3.399	18.028	1.00	10.60
ATOM	992	CG	LEU	A	169	15.513	2.319	18.742	1.00	11.30
ATOM	993	CD1	LEU	A	169	16.999	2.578	18.525	1.00	12.03
ATOM	994	CD2	LEU	A	169	15.166	2.358	20.234	1.00	9.04
ATOM	995	N	LEU	A	170	12.592	4.872	16.420	1.00	17.54
ATOM	996	CA	LEU	A	170	12.051	6.045	15.752	1.00	17.32
ATOM	997	C	LEU	A	170	10.598	6.259	16.127	1.00	18.92
ATOM	998	O	LEU	A	170	10.169	7.404	16.372	1.00	21.34
ATOM	999	CB	LEU	A	170	12.180	5.926	14.230	1.00	15.04
ATOM	1000	CG	LEU	A	170	13.436	6.497	13.569	1.00	16.49

FIG. 2R

ATOM	1001	CD1	LEU	A	170	13.849	7.801	14.238	1.00	15.81
ATOM	1002	CD2	LEU	A	170	14.565	5.538	13.628	1.00	19.02
ATOM	1003	N	TYR	A	171	9.842	5.163	16.177	1.00	16.52
ATOM	1004	CA	TYR	A	171	8.416	5.198	16.541	1.00	14.86
ATOM	1005	C	TYR	A	171	8.178	5.805	17.964	1.00	12.63
ATOM	1006	O	TYR	A	171	7.165	6.463	18.240	1.00	9.35
ATOM	1007	CB	TYR	A	171	7.853	3.760	16.462	1.00	9.52
ATOM	1008	CG	TYR	A	171	6.505	3.587	17.120	1.00	4.84
ATOM	1009	CD1	TYR	A	171	5.366	4.162	16.584	1.00	5.95
ATOM	1010	CD2	TYR	A	171	6.389	2.939	18.338	1.00	6.08
ATOM	1011	CE1	TYR	A	171	4.153	4.109	17.246	1.00	4.75
ATOM	1012	CE2	TYR	A	171	5.173	2.891	19.010	1.00	3.46
ATOM	1013	CZ	TYR	A	171	4.065	3.479	18.458	1.00	3.67
ATOM	1014	OH	TYR	A	171	2.864	3.467	19.127	1.00	8.68
ATOM	1015	N	GLN	A	172	9.099	5.503	18.875	1.00	14.87
ATOM	1016	CA	GLN	A	172	9.030	5.963	20.249	1.00	14.72
ATOM	1017	C	GLN	A	172	9.357	7.460	20.384	1.00	14.62
ATOM	1018	O	GLN	A	172	8.767	8.168	21.226	1.00	12.03
ATOM	1019	CB	GLN	A	172	9.956	5.107	21.112	1.00	14.49
ATOM	1020	CG	GLN	A	172	9.403	3.735	21.412	1.00	15.16
ATOM	1021	CD	GLN	A	172	10.305	2.948	22.334	1.00	15.71
ATOM	1022	OE1	GLN	A	172	10.043	2.854	23.533	1.00	13.46
ATOM	1023	NE2	GLN	A	172	11.376	2.364	21.776	1.00	16.53
ATOM	1024	N	MET	A	173	10.303	7.915	19.555	1.00	16.38
ATOM	1025	CA	MET	A	173	10.719	9.307	19.498	1.00	16.01
ATOM	1026	C	MET	A	173	9.526	10.136	19.014	1.00	18.08
ATOM	1027	O	MET	A	173	9.413	11.309	19.365	1.00	21.67
ATOM	1028	CB	MET	A	173	11.879	9.495	18.527	1.00	13.67
ATOM	1029	CG	MET	A	173	13.172	8.828	18.907	1.00	12.28
ATOM	1030	SD	MET	A	173	14.465	9.098	17.676	1.00	18.92
ATOM	1031	CE	MET	A	173	15.565	7.839	17.983	1.00	11.44
ATOM	1032	N	LEU	A	174	8.646	9.524	18.210	1.00	15.57
ATOM	1033	CA	LEU	A	174	7.453	10.191	17.696	1.00	12.84
ATOM	1034	C	LEU	A	174	6.272	10.134	18.663	1.00	14.56
ATOM	1035	O	LEU	A	174	5.423	11.013	18.649	1.00	14.93
ATOM	1036	CB	LEU	A	174	7.007	9.591	16.359	1.00	15.43
ATOM	1037	CG	LEU	A	174	7.818	9.716	15.061	1.00	19.44
ATOM	1038	CD1	LEU	A	174	7.204	8.752	13.999	1.00	14.81
ATOM	1039	CD2	LEU	A	174	7.844	11.174	14.554	1.00	14.90
ATOM	1040	N	CYS	A	175	6.131	9.043	19.407	1.00	14.52
ATOM	1041	CA	CYS	A	175	5.054	8.950	20.377	1.00	16.46
ATOM	1042	C	CYS	A	175	5.372	9.995	21.451	1.00	17.66
ATOM	1043	O	CYS	A	175	4.485	10.702	21.915	1.00	20.36
ATOM	1044	CB	CYS	A	175	5.036	7.567	21.033	1.00	19.53
ATOM	1045	SG	CYS	A	175	4.596	6.190	19.979	1.00	20.01
ATOM	1046	N	GLY	A	176	6.645	10.052	21.854	1.00	16.83
ATOM	1047	CA	GLY	A	176	7.097	11.000	22.855	1.00	19.04
ATOM	1048	C	GLY	A	176	6.873	12.419	22.385	1.00	18.61
ATOM	1049	O	GLY	A	176	6.121	13.169	23.006	1.00	20.79
ATOM	1050	N	ILE	A	177	7.450	12.761	21.238	1.00	20.33
ATOM	1051	CA	ILE	A	177	7.296	14.098	20.661	1.00	20.67
ATOM	1052	C	ILE	A	177	5.822	14.417	20.428	1.00	21.19
ATOM	1053	O	ILE	A	177	5.403	15.566	20.545	1.00	25.02
ATOM	1054	CB	ILE	A	177	8.080	14.265	19.322	1.00	20.27
ATOM	1055	CG1	ILE	A	177	9.566	14.447	19.595	1.00	16.70
ATOM	1056	CG2	ILE	A	177	7.588	15.460	18.569	1.00	16.17
ATOM	1057	CD1	ILE	A	177	9.865	15.683	20.397	1.00	22.15
ATOM	1058	N	LYS	A	178	5.011	13.405	20.170	1.00	20.18
ATOM	1059	CA	LYS	A	178	3.603	13.659	19.953	1.00	20.86

FIG. 2S

ATOM	1060	C	LYS	A	178	3.021	14.122	21.278	1.00	21.67
ATOM	1061	O	LYS	A	178	2.264	15.090	21.324	1.00	22.72
ATOM	1062	CB	LYS	A	178	2.882	12.385	19.453	1.00	22.57
ATOM	1063	CG	LYS	A	178	1.342	12.466	19.385	1.00	23.42
ATOM	1064	CD	LYS	A	178	0.831	13.317	18.231	1.00	23.55
ATOM	1065	CE	LYS	A	178	-0.664	13.641	18.369	1.00	25.60
ATOM	1066	NZ	LYS	A	178	-0.937	14.847	19.258	1.00	30.22
ATOM	1067	N	HIS	A	179	3.438	13.470	22.360	1.00	21.34
ATOM	1068	CA	HIS	A	179	2.928	13.780	23.692	1.00	19.74
ATOM	1069	C	HIS	A	179	3.300	15.203	24.066	1.00	20.78
ATOM	1070	O	HIS	A	179	2.459	16.017	24.469	1.00	19.29
ATOM	1071	CB	HIS	A	179	3.518	12.803	24.714	1.00	19.07
ATOM	1072	CG	HIS	A	179	2.790	12.784	26.024	1.00	18.62
ATOM	1073	ND1	HIS	A	179	1.458	12.440	26.133	1.00	19.00
ATOM	1074	CD2	HIS	A	179	3.217	13.032	27.281	1.00	16.10
ATOM	1075	CE1	HIS	A	179	1.098	12.478	27.400	1.00	16.49
ATOM	1076	NE2	HIS	A	179	2.148	12.831	28.118	1.00	16.27
ATOM	1077	N	LEU	A	180	4.574	15.498	23.882	1.00	22.10
ATOM	1078	CA	LEU	A	180	5.122	16.807	24.166	1.00	22.49
ATOM	1079	C	LEU	A	180	4.254	17.916	23.528	1.00	24.20
ATOM	1080	O	LEU	A	180	3.833	18.847	24.212	1.00	26.51
ATOM	1081	CB	LEU	A	180	6.556	16.849	23.643	1.00	14.03
ATOM	1082	CG	LEU	A	180	7.665	16.998	24.674	1.00	12.96
ATOM	1083	CD1	LEU	A	180	7.396	16.215	25.911	1.00	14.52
ATOM	1084	CD2	LEU	A	180	8.981	16.643	24.071	1.00	11.14
ATOM	1085	N	HIS	A	181	3.888	17.745	22.258	1.00	26.53
ATOM	1086	CA	HIS	A	181	3.090	18.731	21.535	1.00	24.04
ATOM	1087	C	HIS	A	181	1.671	18.824	22.031	1.00	24.90
ATOM	1088	O	HIS	A	181	1.023	19.864	21.866	1.00	25.57
ATOM	1089	CB	HIS	A	181	3.057	18.398	20.046	1.00	22.90
ATOM	1090	CG	HIS	A	181	4.388	18.473	19.384	1.00	19.53
ATOM	1091	ND1	HIS	A	181	4.648	17.875	18.171	1.00	20.99
ATOM	1092	CD2	HIS	A	181	5.533	19.087	19.745	1.00	20.47
ATOM	1093	CE1	HIS	A	181	5.891	18.127	17.812	1.00	19.62
ATOM	1094	NE2	HIS	A	181	6.452	18.863	18.750	1.00	21.72
ATOM	1095	N	SER	A	182	1.176	17.745	22.634	1.00	26.36
ATOM	1096	CA	SER	A	182	-0.200	17.714	23.121	1.00	25.41
ATOM	1097	C	SER	A	182	-0.377	18.611	24.326	1.00	23.05
ATOM	1098	O	SER	A	182	-1.474	19.099	24.578	1.00	23.50
ATOM	1099	CB	SER	A	182	-0.671	16.281	23.410	1.00	25.02
ATOM	1100	OG	SER	A	182	0.088	15.684	24.441	1.00	22.43
ATOM	1101	N	ALA	A	183	0.730	18.860	25.026	1.00	25.30
ATOM	1102	CA	ALA	A	183	0.761	19.724	26.222	1.00	23.47
ATOM	1103	C	ALA	A	183	1.369	21.090	25.884	1.00	21.12
ATOM	1104	O	ALA	A	183	1.817	21.832	26.757	1.00	19.62
ATOM	1105	CB	ALA	A	183	1.541	19.042	27.368	1.00	23.94
ATOM	1106	N	GLY	A	184	1.393	21.394	24.591	1.00	21.16
ATOM	1107	CA	GLY	A	184	1.906	22.660	24.117	1.00	19.99
ATOM	1108	C	GLY	A	184	3.398	22.801	24.158	1.00	20.18
ATOM	1109	O	GLY	A	184	3.924	23.884	23.952	1.00	27.13
ATOM	1110	N	ILE	A	185	4.092	21.709	24.398	1.00	19.83
ATOM	1111	CA	ILE	A	185	5.534	21.738	24.460	1.00	17.77
ATOM	1112	C	ILE	A	185	6.106	21.419	23.079	1.00	19.73
ATOM	1113	O	ILE	A	185	5.691	20.448	22.451	1.00	20.08
ATOM	1114	CB	ILE	A	185	6.044	20.679	25.507	1.00	16.71
ATOM	1115	CG1	ILE	A	185	5.433	20.950	26.874	1.00	15.07
ATOM	1116	CG2	ILE	A	185	7.557	20.723	25.644	1.00	15.10
ATOM	1117	CD1	ILE	A	185	5.470	19.754	27.801	1.00	17.54
ATOM	1118	N	ILE	A	186	6.983	22.285	22.573	1.00	20.86

FIG. 2T

ATOM	1119	CA	ILE	A	186	7.665	22.044	21.306	1.00	22.18
ATOM	1120	C	ILE	A	186	9.151	22.138	21.659	1.00	21.75
ATOM	1121	O	ILE	A	186	9.658	23.179	22.081	1.00	27.20
ATOM	1122	CB	ILE	A	186	7.214	23.015	20.153	1.00	24.64
ATOM	1123	CG1	ILE	A	186	5.732	22.796	19.843	1.00	23.72
ATOM	1124	CG2	ILE	A	186	8.000	22.750	18.861	1.00	17.81
ATOM	1125	CD1	ILE	A	186	5.268	23.484	18.577	1.00	27.86
ATOM	1126	N	HIS	A	187	9.799	20.981	21.587	1.00	19.52
ATOM	1127	CA	HIS	A	187	11.207	20.786	21.931	1.00	18.54
ATOM	1128	C	HIS	A	187	12.210	21.732	21.268	1.00	18.78
ATOM	1129	O	HIS	A	187	12.834	22.542	21.932	1.00	20.80
ATOM	1130	CB	HIS	A	187	11.576	19.330	21.601	1.00	10.73
ATOM	1131	CG	HIS	A	187	12.629	18.740	22.481	1.00	3.47
ATOM	1132	ND1	HIS	A	187	13.960	19.081	22.396	1.00	6.36
ATOM	1133	CD2	HIS	A	187	12.555	17.774	23.424	1.00	2.00
ATOM	1134	CE1	HIS	A	187	14.661	18.349	23.239	1.00	2.00
ATOM	1135	NE2	HIS	A	187	13.829	17.547	23.872	1.00	2.00
ATOM	1136	N	ARG	A	188	12.411	21.534	19.968	1.00	19.66
ATOM	1137	CA	ARG	A	188	13.348	22.293	19.146	1.00	16.52
ATOM	1138	C	ARG	A	188	14.836	22.006	19.298	1.00	15.80
ATOM	1139	O	ARG	A	188	15.639	22.568	18.560	1.00	15.23
ATOM	1140	CB	ARG	A	188	13.045	23.789	19.177	1.00	14.87
ATOM	1141	CG	ARG	A	188	11.829	24.129	18.351	1.00	18.15
ATOM	1142	CD	ARG	A	188	10.890	25.057	19.053	1.00	22.53
ATOM	1143	NE	ARG	A	188	11.487	26.372	19.211	1.00	27.78
ATOM	1144	CZ	ARG	A	188	11.650	26.963	20.387	1.00	33.29
ATOM	1145	NH1	ARG	A	188	11.251	26.333	21.491	1.00	41.12
ATOM	1146	NH2	ARG	A	188	12.242	28.151	20.473	1.00	27.48
ATOM	1147	N	ASP	A	189	15.222	21.138	20.236	1.00	15.50
ATOM	1148	CA	ASP	A	189	16.638	20.780	20.379	1.00	13.83
ATOM	1149	C	ASP	A	189	16.861	19.314	20.692	1.00	15.26
ATOM	1150	O	ASP	A	189	17.738	18.965	21.453	1.00	16.82
ATOM	1151	CB	ASP	A	189	17.373	21.650	21.396	1.00	14.00
ATOM	1152	CG	ASP	A	189	18.880	21.538	21.266	1.00	12.97
ATOM	1153	OD1	ASP	A	189	19.366	21.256	20.151	1.00	16.34
ATOM	1154	OD2	ASP	A	189	19.595	21.720	22.270	1.00	20.60
ATOM	1155	N	LEU	A	190	16.061	18.458	20.071	1.00	18.38
ATOM	1156	CA	LEU	A	190	16.156	17.017	20.260	1.00	17.27
ATOM	1157	C	LEU	A	190	17.489	16.511	19.704	1.00	17.59
ATOM	1158	O	LEU	A	190	17.781	16.718	18.529	1.00	19.56
ATOM	1159	CB	LEU	A	190	15.028	16.339	19.497	1.00	18.00
ATOM	1160	CG	LEU	A	190	14.039	15.459	20.236	1.00	19.47
ATOM	1161	CD1	LEU	A	190	13.442	14.528	19.206	1.00	24.47
ATOM	1162	CD2	LEU	A	190	14.706	14.649	21.343	1.00	17.28
ATOM	1163	N	LYS	A	191	18.316	15.907	20.550	1.00	14.84
ATOM	1164	CA	LYS	A	191	19.586	15.365	20.112	1.00	13.20
ATOM	1165	C	LYS	A	191	19.767	13.973	20.714	1.00	15.81
ATOM	1166	O	LYS	A	191	19.235	13.671	21.772	1.00	15.29
ATOM	1167	CB	LYS	A	191	20.744	16.280	20.480	1.00	11.69
ATOM	1168	CG	LYS	A	191	20.654	16.909	21.812	1.00	15.09
ATOM	1169	CD	LYS	A	191	21.862	17.810	22.036	1.00	22.46
ATOM	1170	CE	LYS	A	191	21.492	19.282	22.275	1.00	25.84
ATOM	1171	NZ	LYS	A	191	22.702	20.087	22.680	1.00	33.38
ATOM	1172	N	PRO	A	192	20.533	13.105	20.049	1.00	19.16
ATOM	1173	CA	PRO	A	192	20.703	11.735	20.539	1.00	17.61
ATOM	1174	C	PRO	A	192	21.294	11.682	21.964	1.00	14.91
ATOM	1175	O	PRO	A	192	21.023	10.783	22.747	1.00	13.47
ATOM	1176	CB	PRO	A	192	21.619	10.990	19.574	1.00	17.17
ATOM	1177	CG	PRO	A	192	22.287	12.021	18.680	1.00	19.74

FIG. 2U

ATOM	1178	CD	PRO	A	192	21.274	13.253	18.799	1.00	19.71
ATOM	1179	N	SER	A	193	22.168	12.663	22.270	1.00	14.53
ATOM	1180	CA	SER	A	193	22.816	12.651	23.581	1.00	14.67
ATOM	1181	C	SER	A	193	21.814	12.886	24.719	1.00	14.06
ATOM	1182	O	SER	A	193	22.076	12.622	25.884	1.00	17.22
ATOM	1183	CB	SER	A	193	23.900	13.738	23.598	1.00	10.46
ATOM	1184	OG	SER	A	193	23.286	15.023	23.592	1.00	15.44
ATOM	1185	N	ASN	A	194	20.642	13.441	24.347	1.00	13.38
ATOM	1186	CA	ASN	A	194	19.607	13.678	25.352	1.00	14.45
ATOM	1187	C	ASN	A	194	18.522	12.602	25.303	1.00	13.47
ATOM	1188	O	ASN	A	194	17.419	12.761	25.804	1.00	14.24
ATOM	1189	CB	ASN	A	194	18.994	15.055	25.096	1.00	20.06
ATOM	1190	CG	ASN	A	194	19.928	16.118	25.614	1.00	18.16
ATOM	1191	OD1	ASN	A	194	19.977	17.242	25.116	1.00	18.33
ATOM	1192	ND2	ASN	A	194	20.694	15.740	26.648	1.00	19.86
ATOM	1193	N	ILE	A	195	18.864	11.489	24.626	1.00	13.73
ATOM	1194	CA	ILE	A	195	17.953	10.351	24.592	1.00	11.13
ATOM	1195	C	ILE	A	195	18.644	9.085	25.085	1.00	10.38
ATOM	1196	O	ILE	A	195	19.810	8.829	24.817	1.00	7.75
ATOM	1197	CB	ILE	A	195	17.484	10.152	23.154	1.00	13.28
ATOM	1198	CG1	ILE	A	195	16.719	11.378	22.669	1.00	13.74
ATOM	1199	CG2	ILE	A	195	16.533	8.942	23.077	1.00	10.53
ATOM	1200	CD1	ILE	A	195	16.405	11.306	21.176	1.00	15.83
ATOM	1201	N	VAL	A	196	17.892	8.297	25.865	1.00	10.18
ATOM	1202	CA	VAL	A	196	18.456	7.062	26.387	1.00	6.55
ATOM	1203	C	VAL	A	196	17.579	5.860	26.027	1.00	5.22
ATOM	1204	O	VAL	A	196	16.385	5.983	25.788	1.00	2.00
ATOM	1205	CB	VAL	A	196	18.555	7.195	27.907	1.00	3.87
ATOM	1206	CG1	VAL	A	196	19.804	7.994	28.284	1.00	2.00
ATOM	1207	CG2	VAL	A	196	17.328	7.908	28.440	1.00	2.00
ATOM	1208	N	VAL	A	197	18.236	4.710	26.026	1.00	13.84
ATOM	1209	CA	VAL	A	197	17.573	3.445	25.675	1.00	15.82
ATOM	1210	C	VAL	A	197	17.879	2.253	26.626	1.00	17.01
ATOM	1211	O	VAL	A	197	18.991	2.119	27.152	1.00	17.00
ATOM	1212	CB	VAL	A	197	18.008	3.045	24.251	1.00	16.24
ATOM	1213	CG1	VAL	A	197	17.798	4.222	23.286	1.00	12.09
ATOM	1214	CG2	VAL	A	197	19.488	2.637	24.266	1.00	10.94
ATOM	1215	N	LYS	A	198	16.885	1.405	26.856	1.00	15.55
ATOM	1216	CA	LYS	A	198	17.107	0.232	27.681	1.00	20.15
ATOM	1217	C	LYS	A	198	17.396	-0.899	26.689	1.00	21.33
ATOM	1218	O	LYS	A	198	16.948	-0.853	25.554	1.00	23.61
ATOM	1219	CB	LYS	A	198	15.901	-0.075	28.585	1.00	21.73
ATOM	1220	CG	LYS	A	198	16.229	-1.021	29.758	1.00	22.90
ATOM	1221	CD	LYS	A	198	15.484	-0.642	31.034	1.00	19.80
ATOM	1222	CE	LYS	A	198	14.013	-0.900	30.851	1.00	24.82
ATOM	1223	NZ	LYS	A	198	13.122	-0.205	31.823	1.00	28.63
ATOM	1224	N	SER	A	199	18.175	-1.888	27.110	1.00	21.24
ATOM	1225	CA	SER	A	199	18.575	-3.002	26.260	1.00	21.97
ATOM	1226	C	SER	A	199	17.421	-3.694	25.529	1.00	19.69
ATOM	1227	O	SER	A	199	17.620	-4.306	24.490	1.00	21.65
ATOM	1228	CB	SER	A	199	19.448	-4.005	27.040	1.00	24.60
ATOM	1229	OG	SER	A	199	18.742	-4.608	28.113	1.00	28.88
ATOM	1230	N	ASP	A	200	16.210	-3.541	26.045	1.00	20.67
ATOM	1231	CA	ASP	A	200	15.024	-4.119	25.418	1.00	20.33
ATOM	1232	C	ASP	A	200	14.504	-3.197	24.316	1.00	21.43
ATOM	1233	O	ASP	A	200	13.393	-3.377	23.816	1.00	21.33
ATOM	1234	CB	ASP	A	200	13.915	-4.434	26.458	1.00	22.61
ATOM	1235	CG	ASP	A	200	13.503	-3.219	27.329	1.00	27.20
ATOM	1236	OD1	ASP	A	200	14.060	-2.103	27.160	1.00	28.10

FIG. 2V

ATOM	1237	OD2	ASP	A	200	12.593	-3.382	28.186	1.00	26.74
ATOM	1238	N	CYS	A	201	15.317	-2.198	23.967	1.00	21.96
ATOM	1239	CA	CYS	A	201	15.007	-1.218	22.926	1.00	22.56
ATOM	1240	C	CYS	A	201	14.060	-0.069	23.309	1.00	22.96
ATOM	1241	O	CYS	A	201	13.800	0.829	22.496	1.00	22.78
ATOM	1242	CB	CYS	A	201	14.463	-1.936	21.689	1.00	23.72
ATOM	1243	SG	CYS	A	201	14.878	-1.138	20.161	1.00	20.78
ATOM	1244	N	THR	A	202	13.501	-0.117	24.516	1.00	21.58
ATOM	1245	CA	THR	A	202	12.588	0.931	24.960	1.00	18.40
ATOM	1246	C	THR	A	202	13.402	2.212	25.086	1.00	17.04
ATOM	1247	O	THR	A	202	14.630	2.158	25.289	1.00	12.40
ATOM	1248	CB	THR	A	202	11.768	0.539	26.245	1.00	21.86
ATOM	1249	OG1	THR	A	202	12.641	0.277	27.353	1.00	22.39
ATOM	1250	CG2	THR	A	202	10.927	-0.699	25.955	1.00	17.91
ATOM	1251	N	LEU	A	203	12.737	3.352	24.882	1.00	15.72
ATOM	1252	CA	LEU	A	203	13.443	4.638	24.849	1.00	15.61
ATOM	1253	C	LEU	A	203	12.799	5.783	25.608	1.00	12.44
ATOM	1254	O	LEU	A	203	11.594	5.818	25.771	1.00	14.74
ATOM	1255	CB	LEU	A	203	13.593	5.026	23.370	1.00	13.34
ATOM	1256	CG	LEU	A	203	14.053	6.392	22.862	1.00	13.72
ATOM	1257	CD1	LEU	A	203	14.565	6.168	21.459	1.00	13.05
ATOM	1258	CD2	LEU	A	203	12.885	7.421	22.904	1.00	7.57
ATOM	1259	N	LYS	A	204	13.603	6.768	25.986	1.00	12.90
ATOM	1260	CA	LYS	A	204	13.083	7.931	26.703	1.00	12.48
ATOM	1261	C	LYS	A	204	13.830	9.241	26.369	1.00	13.43
ATOM	1262	O	LYS	A	204	15.060	9.254	26.260	1.00	15.08
ATOM	1263	CB	LYS	A	204	13.149	7.676	28.215	1.00	12.82
ATOM	1264	CG	LYS	A	204	12.225	6.562	28.723	1.00	12.27
ATOM	1265	CD	LYS	A	204	12.577	6.186	30.146	1.00	16.47
ATOM	1266	CE	LYS	A	204	11.544	5.243	30.730	1.00	13.58
ATOM	1267	NZ	LYS	A	204	10.268	5.952	31.015	1.00	18.54
ATOM	1268	N	ILE	A	205	13.084	10.323	26.134	1.00	15.04
ATOM	1269	CA	ILE	A	205	13.696	11.626	25.872	1.00	15.29
ATOM	1270	C	ILE	A	205	13.928	12.237	27.262	1.00	14.25
ATOM	1271	O	ILE	A	205	13.017	12.326	28.070	1.00	14.09
ATOM	1272	CB	ILE	A	205	12.756	12.543	25.062	1.00	18.47
ATOM	1273	CG1	ILE	A	205	12.417	11.891	23.718	1.00	19.00
ATOM	1274	CG2	ILE	A	205	13.418	13.919	24.842	1.00	17.93
ATOM	1275	CD1	ILE	A	205	11.256	12.571	22.962	1.00	14.77
ATOM	1276	N	LEU	A	206	15.144	12.664	27.544	1.00	15.06
ATOM	1277	CA	LEU	A	206	15.450	13.206	28.860	1.00	15.79
ATOM	1278	C	LEU	A	206	15.181	14.704	29.121	1.00	20.48
ATOM	1279	O	LEU	A	206	15.034	15.108	30.287	1.00	20.24
ATOM	1280	CB	LEU	A	206	16.898	12.901	29.201	1.00	11.74
ATOM	1281	CG	LEU	A	206	17.372	11.468	29.137	1.00	11.09
ATOM	1282	CD1	LEU	A	206	18.854	11.500	29.409	1.00	8.65
ATOM	1283	CD2	LEU	A	206	16.585	10.585	30.134	1.00	7.68
ATOM	1284	N	ASP	A	207	15.091	15.521	28.062	1.00	21.50
ATOM	1285	CA	ASP	A	207	14.878	16.961	28.234	1.00	17.68
ATOM	1286	C	ASP	A	207	13.672	17.490	27.490	1.00	18.35
ATOM	1287	O	ASP	A	207	13.002	16.735	26.789	1.00	20.08
ATOM	1288	CB	ASP	A	207	16.133	17.713	27.797	1.00	21.59
ATOM	1289	CG	ASP	A	207	16.380	17.644	26.273	1.00	29.58
ATOM	1290	OD1	ASP	A	207	15.808	16.778	25.550	1.00	31.34
ATOM	1291	OD2	ASP	A	207	17.184	18.471	25.799	1.00	31.59
ATOM	1292	N	PHE	A	208	13.433	18.799	27.611	1.00	15.65
ATOM	1293	CA	PHE	A	208	12.293	19.456	26.958	1.00	13.93
ATOM	1294	C	PHE	A	208	12.623	20.581	25.940	1.00	12.22
ATOM	1295	O	PHE	A	208	11.741	21.317	25.523	1.00	11.22

FIG. 2W

ATOM	1296	CB	PHE	A	208	11.300	19.929	28.019	1.00	12.75
ATOM	1297	CG	PHE	A	208	10.723	18.812	28.840	1.00	17.68
ATOM	1298	CD1	PHE	A	208	11.314	18.431	30.045	1.00	19.52
ATOM	1299	CD2	PHE	A	208	9.592	18.131	28.405	1.00	18.93
ATOM	1300	CE1	PHE	A	208	10.791	17.383	30.799	1.00	20.99
ATOM	1301	CE2	PHE	A	208	9.056	17.082	29.145	1.00	16.66
ATOM	1302	CZ	PHE	A	208	9.658	16.704	30.349	1.00	19.20
ATOM	1303	N	GLY	A	209	13.884	20.668	25.524	1.00	12.18
ATOM	1304	CA	GLY	A	209	14.293	21.671	24.553	1.00	20.92
ATOM	1305	C	GLY	A	209	14.480	23.061	25.135	1.00	26.49
ATOM	1306	O	GLY	A	209	14.911	23.199	26.284	1.00	29.37
ATOM	1307	N	LEU	A	210	14.154	24.094	24.355	1.00	27.55
ATOM	1308	CA	LEU	A	210	14.280	25.481	24.814	1.00	26.38
ATOM	1309	C	LEU	A	210	12.963	26.193	24.894	1.00	24.27
ATOM	1310	O	LEU	A	210	11.948	25.683	24.436	1.00	22.45
ATOM	1311	CB	LEU	A	210	15.227	26.293	23.931	1.00	26.72
ATOM	1312	CG	LEU	A	210	15.635	25.794	22.557	1.00	22.25
ATOM	1313	CD1	LEU	A	210	16.559	24.611	22.704	1.00	24.06
ATOM	1314	CD2	LEU	A	210	14.405	25.463	21.764	1.00	21.49
ATOM	1315	N	ALA	A	211	12.996	27.391	25.474	1.00	25.71
ATOM	1316	CA	ALA	A	211	11.805	28.209	25.631	1.00	25.90
ATOM	1317	C	ALA	A	211	11.182	28.524	24.272	1.00	27.49
ATOM	1318	O	ALA	A	211	9.971	28.839	24.259	1.00	30.18
ATOM	1319	CB	ALA	A	211	12.162	29.490	26.358	1.00	28.03
ATOM	1320	N	THR	A	217	21.725	33.846	24.927	1.00	39.03
ATOM	1321	CA	THR	A	217	21.912	33.243	26.279	1.00	40.85
ATOM	1322	C	THR	A	217	23.409	33.084	26.550	1.00	40.53
ATOM	1323	O	THR	A	217	24.163	32.693	25.645	1.00	41.22
ATOM	1324	CB	THR	A	217	21.211	31.869	26.349	1.00	42.09
ATOM	1325	OG1	THR	A	217	21.739	31.013	25.325	1.00	43.36
ATOM	1326	CG2	THR	A	217	19.702	32.032	26.133	1.00	42.14
ATOM	1327	N	PHE	A	218	23.835	33.382	27.782	1.00	38.09
ATOM	1328	CA	PHE	A	218	25.252	33.288	28.137	1.00	35.72
ATOM	1329	C	PHE	A	218	25.639	32.253	29.213	1.00	36.31
ATOM	1330	O	PHE	A	218	24.816	31.823	30.033	1.00	34.01
ATOM	1331	CB	PHE	A	218	25.775	34.666	28.537	1.00	33.12
ATOM	1332	CG	PHE	A	218	27.274	34.800	28.417	1.00	28.01
ATOM	1333	CD1	PHE	A	218	28.028	35.285	29.469	1.00	23.49
ATOM	1334	CD2	PHE	A	218	27.920	34.458	27.244	1.00	26.30
ATOM	1335	CE1	PHE	A	218	29.397	35.418	29.364	1.00	23.12
ATOM	1336	CE2	PHE	A	218	29.297	34.589	27.125	1.00	25.69
ATOM	1337	CZ	PHE	A	218	30.037	35.076	28.192	1.00	24.92
ATOM	1338	N	MET	A	219	26.913	31.875	29.184	1.00	37.55
ATOM	1339	CA	MET	A	219	27.485	30.905	30.098	1.00	37.63
ATOM	1340	C	MET	A	219	29.007	31.004	30.025	1.00	35.79
ATOM	1341	O	MET	A	219	29.556	31.607	29.105	1.00	33.20
ATOM	1342	CB	MET	A	219	27.068	29.491	29.673	1.00	41.36
ATOM	1343	CG	MET	A	219	25.906	28.887	30.439	1.00	44.77
ATOM	1344	SD	MET	A	219	26.233	27.124	30.636	1.00	50.51
ATOM	1345	CE	MET	A	219	24.764	26.343	29.870	1.00	48.78
ATOM	1346	N	MET	A	220	29.679	30.412	31.006	1.00	38.17
ATOM	1347	CA	MET	A	220	31.138	30.400	31.048	1.00	40.05
ATOM	1348	C	MET	A	220	31.621	28.954	30.873	1.00	42.28
ATOM	1349	O	MET	A	220	32.507	28.471	31.587	1.00	40.47
ATOM	1350	CB	MET	A	220	31.651	31.017	32.357	1.00	40.79
ATOM	1351	CG	MET	A	220	31.507	32.545	32.443	1.00	34.52
ATOM	1352	SD	MET	A	220	32.795	33.453	31.587	1.00	36.04
ATOM	1353	CE	MET	A	220	33.047	34.823	32.693	1.00	36.91
ATOM	1354	N	THR	A	221	31.059	28.309	29.853	1.00	45.09

FIG. 2X

ATOM	1355	CA	THR	A	221	31.345	26.924	29.501	1.00	47.82
ATOM	1356	C	THR	A	221	32.628	26.629	28.710	1.00	48.65
ATOM	1357	O	THR	A	221	33.056	27.421	27.855	1.00	46.82
ATOM	1358	CB	THR	A	221	30.188	26.313	28.685	1.00	48.78
ATOM	1359	OG1	THR	A	221	30.476	24.938	28.415	1.00	50.50
ATOM	1360	CG2	THR	A	221	30.014	27.066	27.349	1.00	47.96
ATOM	1361	N	PRO	A	222	33.262	25.480	29.019	1.00	50.08
ATOM	1362	CA	PRO	A	222	34.496	24.999	28.379	1.00	49.33
ATOM	1363	C	PRO	A	222	34.168	24.251	27.066	1.00	49.92
ATOM	1364	O	PRO	A	222	35.051	24.019	26.210	1.00	49.18
ATOM	1365	CB	PRO	A	222	35.078	24.038	29.437	1.00	49.23
ATOM	1366	CG	PRO	A	222	34.485	24.523	30.752	1.00	46.35
ATOM	1367	CD	PRO	A	222	33.064	24.795	30.320	1.00	49.40
ATOM	1368	N	TYR	A	223	32.896	23.879	26.917	1.00	48.31
ATOM	1369	CA	TYR	A	223	32.430	23.153	25.734	1.00	46.87
ATOM	1370	C	TYR	A	223	30.998	23.481	25.293	1.00	45.04
ATOM	1371	O	TYR	A	223	30.047	23.432	26.080	1.00	42.04
ATOM	1372	CB	TYR	A	223	32.605	21.636	25.916	1.00	49.32
ATOM	1373	CG	TYR	A	223	32.831	21.187	27.343	1.00	50.28
ATOM	1374	CD1	TYR	A	223	34.108	20.822	27.784	1.00	49.70
ATOM	1375	CD2	TYR	A	223	31.769	21.108	28.241	1.00	51.00
ATOM	1376	CE1	TYR	A	223	34.322	20.394	29.088	1.00	50.13
ATOM	1377	CE2	TYR	A	223	31.973	20.677	29.546	1.00	53.18
ATOM	1378	CZ	TYR	A	223	33.251	20.325	29.961	1.00	53.33
ATOM	1379	OH	TYR	A	223	33.447	19.933	31.262	1.00	54.87
ATOM	1380	N	VAL	A	224	30.882	23.786	24.002	1.00	44.41
ATOM	1381	CA	VAL	A	224	29.635	24.157	23.321	1.00	42.98
ATOM	1382	C	VAL	A	224	28.495	23.131	23.349	1.00	41.44
ATOM	1383	O	VAL	A	224	28.700	21.949	23.629	1.00	43.91
ATOM	1384	CB	VAL	A	224	29.915	24.441	21.804	1.00	42.37
ATOM	1385	CG1	VAL	A	224	30.677	25.739	21.615	1.00	38.65
ATOM	1386	CG2	VAL	A	224	30.709	23.281	21.212	1.00	41.83
ATOM	1387	N	VAL	A	225	27.292	23.596	23.025	1.00	38.56
ATOM	1388	CA	VAL	A	225	26.127	22.725	22.943	1.00	36.29
ATOM	1389	C	VAL	A	225	26.143	22.062	21.549	1.00	35.78
ATOM	1390	O	VAL	A	225	26.917	22.446	20.678	1.00	37.18
ATOM	1391	CB	VAL	A	225	24.808	23.519	23.095	1.00	34.26
ATOM	1392	CG1	VAL	A	225	24.687	24.060	24.485	1.00	35.01
ATOM	1393	CG2	VAL	A	225	24.755	24.650	22.095	1.00	32.35
ATOM	1394	N	THR	A	226	25.302	21.061	21.341	1.00	34.31
ATOM	1395	CA	THR	A	226	25.249	20.390	20.051	1.00	30.66
ATOM	1396	C	THR	A	226	24.110	21.025	19.276	1.00	27.91
ATOM	1397	O	THR	A	226	22.986	21.086	19.767	1.00	28.96
ATOM	1398	CB	THR	A	226	24.978	18.896	20.233	1.00	31.72
ATOM	1399	OG1	THR	A	226	26.066	18.305	20.955	1.00	34.08
ATOM	1400	CG2	THR	A	226	24.793	18.203	18.893	1.00	32.43
ATOM	1401	N	ARG	A	227	24.394	21.484	18.062	1.00	25.75
ATOM	1402	CA	ARG	A	227	23.378	22.135	17.243	1.00	22.62
ATOM	1403	C	ARG	A	227	23.056	21.467	15.895	1.00	20.44
ATOM	1404	O	ARG	A	227	22.197	21.943	15.163	1.00	17.13
ATOM	1405	CB	ARG	A	227	23.785	23.589	17.021	1.00	23.83
ATOM	1406	CG	ARG	A	227	25.284	23.761	16.796	1.00	29.07
ATOM	1407	CD	ARG	A	227	25.649	25.158	16.294	1.00	31.42
ATOM	1408	NE	ARG	A	227	26.951	25.581	16.797	1.00	32.03
ATOM	1409	CZ	ARG	A	227	27.110	26.308	17.898	1.00	34.19
ATOM	1410	NH1	ARG	A	227	26.044	26.693	18.591	1.00	34.90
ATOM	1411	NH2	ARG	A	227	28.330	26.592	18.346	1.00	35.55
ATOM	1412	N	TYR	A	228	23.678	20.320	15.625	1.00	20.52
ATOM	1413	CA	TYR	A	228	23.505	19.574	14.359	1.00	15.46

FIG. 2Y

ATOM	1414	C	TYR	A	228	22.097	19.099	14.023	1.00	14.11
ATOM	1415	O	TYR	A	228	21.764	18.866	12.848	1.00	10.68
ATOM	1416	CB	TYR	A	228	24.418	18.355	14.376	1.00	12.40
ATOM	1417	CG	TYR	A	228	25.780	18.697	14.827	1.00	11.72
ATOM	1418	CD1	TYR	A	228	26.455	17.908	15.734	1.00	16.45
ATOM	1419	CD2	TYR	A	228	26.403	19.830	14.351	1.00	16.21
ATOM	1420	CE1	TYR	A	228	27.717	18.241	16.155	1.00	17.57
ATOM	1421	CE2	TYR	A	228	27.661	20.177	14.761	1.00	20.39
ATOM	1422	CZ	TYR	A	228	28.321	19.384	15.663	1.00	18.76
ATOM	1423	OH	TYR	A	228	29.585	19.751	16.061	1.00	21.49
ATOM	1424	N	TYR	A	229	21.272	18.977	15.058	1.00	11.87
ATOM	1425	CA	TYR	A	229	19.911	18.450	14.918	1.00	7.71
ATOM	1426	C	TYR	A	229	18.831	19.492	14.854	1.00	6.14
ATOM	1427	O	TYR	A	229	17.652	19.167	14.735	1.00	7.31
ATOM	1428	CB	TYR	A	229	19.660	17.434	16.048	1.00	5.39
ATOM	1429	CG	TYR	A	229	20.809	16.455	16.151	1.00	2.00
ATOM	1430	CD1	TYR	A	229	21.961	16.799	16.835	1.00	2.00
ATOM	1431	CD2	TYR	A	229	20.810	15.252	15.434	1.00	2.00
ATOM	1432	CE1	TYR	A	229	23.089	16.004	16.800	1.00	6.24
ATOM	1433	CE2	TYR	A	229	21.957	14.428	15.399	1.00	2.47
ATOM	1434	CZ	TYR	A	229	23.091	14.813	16.080	1.00	6.64
ATOM	1435	OH	TYR	A	229	24.253	14.055	16.090	1.00	9.24
ATOM	1436	N	ARG	A	230	19.253	20.751	14.831	1.00	7.71
ATOM	1437	CA	ARG	A	230	18.322	21.869	14.789	1.00	9.82
ATOM	1438	C	ARG	A	230	17.800	22.111	13.373	1.00	7.41
ATOM	1439	O	ARG	A	230	18.558	22.066	12.417	1.00	9.37
ATOM	1440	CB	ARG	A	230	18.991	23.119	15.368	1.00	11.31
ATOM	1441	CG	ARG	A	230	19.147	23.045	16.877	1.00	13.87
ATOM	1442	CD	ARG	A	230	20.032	24.125	17.445	1.00	18.40
ATOM	1443	NE	ARG	A	230	19.874	24.196	18.899	1.00	19.51
ATOM	1444	CZ	ARG	A	230	20.665	24.879	19.725	1.00	18.86
ATOM	1445	NH1	ARG	A	230	21.703	25.583	19.272	1.00	22.89
ATOM	1446	NH2	ARG	A	230	20.436	24.827	21.024	1.00	14.81
ATOM	1447	N	ALA	A	231	16.501	22.379	13.286	1.00	6.42
ATOM	1448	CA	ALA	A	231	15.803	22.613	12.046	1.00	10.20
ATOM	1449	C	ALA	A	231	16.222	23.941	11.442	1.00	17.23
ATOM	1450	O	ALA	A	231	16.794	24.784	12.138	1.00	22.34
ATOM	1451	CB	ALA	A	231	14.336	22.607	12.290	1.00	4.17
ATOM	1452	N	PRO	A	232	15.987	24.141	10.126	1.00	18.56
ATOM	1453	CA	PRO	A	232	16.349	25.392	9.446	1.00	17.77
ATOM	1454	C	PRO	A	232	15.590	26.590	10.010	1.00	16.05
ATOM	1455	O	PRO	A	232	16.117	27.689	10.069	1.00	14.76
ATOM	1456	CB	PRO	A	232	15.992	25.094	7.994	1.00	18.18
ATOM	1457	CG	PRO	A	232	16.259	23.599	7.902	1.00	17.27
ATOM	1458	CD	PRO	A	232	15.575	23.130	9.142	1.00	16.24
ATOM	1459	N	GLU	A	233	14.364	26.347	10.457	1.00	16.97
ATOM	1460	CA	GLU	A	233	13.523	27.366	11.068	1.00	18.57
ATOM	1461	C	GLU	A	233	14.315	27.897	12.248	1.00	21.78
ATOM	1462	O	GLU	A	233	14.164	29.041	12.663	1.00	20.00
ATOM	1463	CB	GLU	A	233	12.264	26.735	11.674	1.00	20.90
ATOM	1464	CG	GLU	A	233	11.251	26.109	10.711	1.00	22.80
ATOM	1465	CD	GLU	A	233	11.250	24.582	10.742	1.00	16.28
ATOM	1466	OE1	GLU	A	233	12.276	23.999	10.381	1.00	16.01
ATOM	1467	OE2	GLU	A	233	10.223	23.969	11.102	1.00	16.64
ATOM	1468	N	VAL	A	234	15.125	27.008	12.824	1.00	22.90
ATOM	1469	CA	VAL	A	234	15.929	27.326	13.987	1.00	18.86
ATOM	1470	C	VAL	A	234	17.315	27.818	13.599	1.00	20.44
ATOM	1471	O	VAL	A	234	17.802	28.788	14.179	1.00	23.91
ATOM	1472	CB	VAL	A	234	16.029	26.091	14.953	1.00	15.02

FIG. 2Z

ATOM	1473	CG1	VAL	A	234	17.058	26.342	16.042	1.00	12.77
ATOM	1474	CG2	VAL	A	234	14.655	25.740	15.535	1.00	7.69
ATOM	1475	N	ILE	A	235	17.942	27.197	12.604	1.00	21.11
ATOM	1476	CA	ILE	A	235	19.272	27.633	12.183	1.00	22.08
ATOM	1477	C	ILE	A	235	19.196	29.001	11.519	1.00	20.93
ATOM	1478	O	ILE	A	235	20.153	29.755	11.543	1.00	20.86
ATOM	1479	CB	ILE	A	235	19.907	26.676	11.153	1.00	22.94
ATOM	1480	CG1	ILE	A	235	20.131	25.300	11.766	1.00	25.93
ATOM	1481	CG2	ILE	A	235	21.231	27.237	10.634	1.00	21.62
ATOM	1482	CD1	ILE	A	235	20.584	24.253	10.739	1.00	27.78
ATOM	1483	N	LEU	A	236	18.038	29.324	10.963	1.00	22.79
ATOM	1484	CA	LEU	A	236	17.861	30.578	10.236	1.00	24.54
ATOM	1485	C	LEU	A	236	16.960	31.601	10.911	1.00	25.47
ATOM	1486	O	LEU	A	236	16.815	32.720	10.442	1.00	26.22
ATOM	1487	CB	LEU	A	236	17.346	30.288	8.822	1.00	21.25
ATOM	1488	CG	LEU	A	236	18.229	29.497	7.860	1.00	16.01
ATOM	1489	CD1	LEU	A	236	17.449	29.276	6.594	1.00	13.14
ATOM	1490	CD2	LEU	A	236	19.524	30.222	7.583	1.00	10.90
ATOM	1491	N	GLY	A	237	16.315	31.198	11.987	1.00	27.03
ATOM	1492	CA	GLY	A	237	15.474	32.124	12.691	1.00	25.56
ATOM	1493	C	GLY	A	237	14.283	32.531	11.869	1.00	29.33
ATOM	1494	O	GLY	A	237	14.386	33.402	10.993	1.00	33.24
ATOM	1495	N	MET	A	238	13.184	31.808	12.070	1.00	24.71
ATOM	1496	CA	MET	A	238	11.924	32.095	11.417	1.00	23.68
ATOM	1497	C	MET	A	238	10.871	31.472	12.289	1.00	22.36
ATOM	1498	O	MET	A	238	11.155	31.078	13.422	1.00	25.57
ATOM	1499	CB	MET	A	238	11.876	31.559	9.980	1.00	24.38
ATOM	1500	CG	MET	A	238	11.982	30.099	9.845	1.00	25.41
ATOM	1501	SD	MET	A	238	12.673	29.699	8.252	1.00	26.30
ATOM	1502	CE	MET	A	238	14.271	29.479	8.685	1.00	25.04
ATOM	1503	N	GLY	A	239	9.638	31.433	11.815	1.00	24.46
ATOM	1504	CA	GLY	A	239	8.589	30.833	12.621	1.00	24.89
ATOM	1505	C	GLY	A	239	8.709	29.320	12.620	1.00	25.61
ATOM	1506	O	GLY	A	239	9.503	28.756	11.863	1.00	22.94
ATOM	1507	N	TYR	A	240	7.930	28.666	13.481	1.00	27.47
ATOM	1508	CA	TYR	A	240	7.944	27.213	13.569	1.00	26.10
ATOM	1509	C	TYR	A	240	6.608	26.662	14.028	1.00	26.67
ATOM	1510	O	TYR	A	240	5.804	27.373	14.650	1.00	27.55
ATOM	1511	CB	TYR	A	240	9.070	26.715	14.514	1.00	27.69
ATOM	1512	CG	TYR	A	240	8.888	27.004	16.000	1.00	24.07
ATOM	1513	CD1	TYR	A	240	7.908	26.360	16.736	1.00	21.50
ATOM	1514	CD2	TYR	A	240	9.666	27.973	16.650	1.00	24.16
ATOM	1515	CE1	TYR	A	240	7.688	26.673	18.083	1.00	26.09
ATOM	1516	CE2	TYR	A	240	9.453	28.300	17.995	1.00	23.28
ATOM	1517	CZ	TYR	A	240	8.454	27.645	18.703	1.00	26.50
ATOM	1518	OH	TYR	A	240	8.158	27.979	20.006	1.00	24.58
ATOM	1519	N	LYS	A	241	6.377	25.396	13.680	1.00	24.48
ATOM	1520	CA	LYS	A	241	5.194	24.662	14.082	1.00	22.48
ATOM	1521	C	LYS	A	241	5.682	23.335	14.673	1.00	21.15
ATOM	1522	O	LYS	A	241	6.874	23.130	14.902	1.00	19.54
ATOM	1523	CB	LYS	A	241	4.222	24.448	12.920	1.00	23.83
ATOM	1524	CG	LYS	A	241	4.858	23.957	11.627	1.00	29.40
ATOM	1525	CD	LYS	A	241	3.786	23.829	10.535	1.00	32.26
ATOM	1526	CE	LYS	A	241	4.387	23.628	9.150	1.00	31.23
ATOM	1527	NZ	LYS	A	241	3.361	23.218	8.134	1.00	31.87
ATOM	1528	N	GLU	A	242	4.755	22.442	14.939	1.00	21.53
ATOM	1529	CA	GLU	A	242	5.078	21.173	15.531	1.00	22.17
ATOM	1530	C	GLU	A	242	6.051	20.289	14.741	1.00	22.70
ATOM	1531	O	GLU	A	242	6.770	19.486	15.340	1.00	22.12

FIG. 2AA

ATOM	1532	CB	GLU	A	242	3.780	20.433	15.830	1.00	27.33
ATOM	1533	CG	GLU	A	242	2.964	21.028	17.004	1.00	31.09
ATOM	1534	CD	GLU	A	242	2.268	22.345	16.700	1.00	29.61
ATOM	1535	OE1	GLU	A	242	2.950	23.358	16.428	1.00	31.84
ATOM	1536	OE2	GLU	A	242	1.027	22.375	16.797	1.00	30.30
ATOM	1537	N	ASN	A	243	6.117	20.447	13.420	1.00	20.30
ATOM	1538	CA	ASN	A	243	7.026	19.607	12.638	1.00	17.12
ATOM	1539	C	ASN	A	243	8.465	20.066	12.598	1.00	15.56
ATOM	1540	O	ASN	A	243	9.279	19.540	11.835	1.00	13.73
ATOM	1541	CB	ASN	A	243	6.481	19.286	11.239	1.00	20.39
ATOM	1542	CG	ASN	A	243	6.467	20.479	10.310	1.00	24.62
ATOM	1543	OD1	ASN	A	243	6.777	21.609	10.706	1.00	26.15
ATOM	1544	ND2	ASN	A	243	6.116	20.227	9.045	1.00	20.34
ATOM	1545	N	VAL	A	244	8.799	21.022	13.457	1.00	15.14
ATOM	1546	CA	VAL	A	244	10.181	21.493	13.565	1.00	14.03
ATOM	1547	C	VAL	A	244	11.041	20.365	14.182	1.00	15.20
ATOM	1548	O	VAL	A	244	12.250	20.263	13.938	1.00	17.55
ATOM	1549	CB	VAL	A	244	10.282	22.752	14.468	1.00	10.37
ATOM	1550	CG1	VAL	A	244	9.645	22.489	15.827	1.00	8.35
ATOM	1551	CG2	VAL	A	244	11.723	23.180	14.615	1.00	10.44
ATOM	1552	N	ASP	A	245	10.396	19.513	14.979	1.00	15.01
ATOM	1553	CA	ASP	A	245	11.075	18.408	15.637	1.00	12.69
ATOM	1554	C	ASP	A	245	11.262	17.229	14.704	1.00	14.61
ATOM	1555	O	ASP	A	245	12.185	16.435	14.878	1.00	18.18
ATOM	1556	CB	ASP	A	245	10.300	18.002	16.892	1.00	13.55
ATOM	1557	CG	ASP	A	245	10.383	19.052	18.000	1.00	4.57
ATOM	1558	OD1	ASP	A	245	11.487	19.485	18.364	1.00	6.51
ATOM	1559	OD2	ASP	A	245	9.330	19.449	18.487	1.00	8.18
ATOM	1560	N	ILE	A	246	10.427	17.165	13.668	1.00	16.73
ATOM	1561	CA	ILE	A	246	10.499	16.125	12.654	1.00	14.31
ATOM	1562	C	ILE	A	246	11.872	16.194	12.007	1.00	15.62
ATOM	1563	O	ILE	A	246	12.530	15.176	11.817	1.00	17.28
ATOM	1564	CB	ILE	A	246	9.393	16.331	11.592	1.00	16.60
ATOM	1565	CG1	ILE	A	246	8.039	15.958	12.185	1.00	9.64
ATOM	1566	CG2	ILE	A	246	9.643	15.492	10.337	1.00	15.94
ATOM	1567	CD1	ILE	A	246	7.967	14.481	12.576	1.00	14.00
ATOM	1568	N	TRP	A	247	12.382	17.403	11.814	1.00	13.79
ATOM	1569	CA	TRP	A	247	13.675	17.550	11.176	1.00	9.95
ATOM	1570	C	TRP	A	247	14.777	16.929	12.008	1.00	8.10
ATOM	1571	O	TRP	A	247	15.716	16.340	11.477	1.00	11.11
ATOM	1572	CB	TRP	A	247	13.959	19.031	10.873	1.00	6.79
ATOM	1573	CG	TRP	A	247	15.372	19.300	10.452	1.00	2.00
ATOM	1574	CD1	TRP	A	247	16.453	19.384	11.270	1.00	2.00
ATOM	1575	CD2	TRP	A	247	15.874	19.456	9.114	1.00	2.85
ATOM	1576	NE1	TRP	A	247	17.596	19.556	10.540	1.00	3.34
ATOM	1577	CE2	TRP	A	247	17.267	19.608	9.212	1.00	2.00
ATOM	1578	CE3	TRP	A	247	15.283	19.479	7.854	1.00	10.65
ATOM	1579	CZ2	TRP	A	247	18.087	19.776	8.088	1.00	6.33
ATOM	1580	CZ3	TRP	A	247	16.096	19.649	6.733	1.00	6.91
ATOM	1581	CH2	TRP	A	247	17.480	19.792	6.857	1.00	7.13
ATOM	1582	N	SER	A	248	14.657	17.072	13.321	1.00	11.35
ATOM	1583	CA	SER	A	248	15.636	16.546	14.280	1.00	8.73
ATOM	1584	C	SER	A	248	15.624	15.021	14.307	1.00	4.47
ATOM	1585	O	SER	A	248	16.670	14.409	14.422	1.00	4.57
ATOM	1586	CB	SER	A	248	15.328	17.100	15.670	1.00	8.62
ATOM	1587	OG	SER	A	248	15.181	18.496	15.578	1.00	7.78
ATOM	1588	N	VAL	A	249	14.433	14.432	14.239	1.00	6.41
ATOM	1589	CA	VAL	A	249	14.248	12.975	14.213	1.00	10.37
ATOM	1590	C	VAL	A	249	14.852	12.455	12.918	1.00	11.86

FIG. 2BB

ATOM	1591	O	VAL	A	249	15.450	11.377	12.894	1.00	15.92
ATOM	1592	CB	VAL	A	249	12.739	12.588	14.254	1.00	9.24
ATOM	1593	CG1	VAL	A	249	12.540	11.091	13.913	1.00	5.95
ATOM	1594	CG2	VAL	A	249	12.132	12.955	15.616	1.00	6.23
ATOM	1595	N	GLY	A	250	14.705	13.246	11.853	1.00	11.69
ATOM	1596	CA	GLY	A	250	15.257	12.897	10.568	1.00	2.74
ATOM	1597	C	GLY	A	250	16.762	12.859	10.608	1.00	7.06
ATOM	1598	O	GLY	A	250	17.374	11.962	10.016	1.00	7.35
ATOM	1599	N	CYS	A	251	17.379	13.821	11.297	1.00	8.01
ATOM	1600	CA	CYS	A	251	18.843	13.892	11.413	1.00	6.02
ATOM	1601	C	CYS	A	251	19.438	12.748	12.224	1.00	6.13
ATOM	1602	O	CYS	A	251	20.620	12.427	12.076	1.00	6.97
ATOM	1603	CB	CYS	A	251	19.295	15.214	12.055	1.00	11.97
ATOM	1604	SG	CYS	A	251	19.073	16.713	11.101	1.00	16.32
ATOM	1605	N	ILE	A	252	18.663	12.224	13.166	1.00	6.86
ATOM	1606	CA	ILE	A	252	19.097	11.104	14.008	1.00	9.70
ATOM	1607	C	ILE	A	252	18.945	9.808	13.172	1.00	6.47
ATOM	1608	O	ILE	A	252	19.870	9.012	13.062	1.00	6.74
ATOM	1609	CB	ILE	A	252	18.204	10.998	15.303	1.00	11.46
ATOM	1610	CG1	ILE	A	252	18.478	12.181	16.277	1.00	6.35
ATOM	1611	CG2	ILE	A	252	18.420	9.645	15.968	1.00	9.02
ATOM	1612	CD1	ILE	A	252	17.278	12.498	17.206	1.00	2.00
ATOM	1613	N	MET	A	253	17.802	9.672	12.520	1.00	4.24
ATOM	1614	CA	MET	A	253	17.524	8.532	11.678	1.00	10.23
ATOM	1615	C	MET	A	253	18.559	8.343	10.566	1.00	13.46
ATOM	1616	O	MET	A	253	18.941	7.219	10.273	1.00	16.51
ATOM	1617	CB	MET	A	253	16.144	8.675	11.061	1.00	10.85
ATOM	1618	CG	MET	A	253	15.864	7.657	9.994	1.00	11.51
ATOM	1619	SD	MET	A	253	14.242	7.881	9.425	1.00	14.35
ATOM	1620	CE	MET	A	253	14.050	6.430	8.483	1.00	14.56
ATOM	1621	N	GLY	A	254	18.977	9.431	9.923	1.00	14.30
ATOM	1622	CA	GLY	A	254	19.964	9.351	8.855	1.00	8.44
ATOM	1623	C	GLY	A	254	21.354	9.118	9.385	1.00	9.82
ATOM	1624	O	GLY	A	254	22.254	8.642	8.672	1.00	9.43
ATOM	1625	N	GLU	A	255	21.582	9.533	10.625	1.00	12.87
ATOM	1626	CA	GLU	A	255	22.873	9.291	11.247	1.00	11.63
ATOM	1627	C	GLU	A	255	22.967	7.802	11.649	1.00	11.63
ATOM	1628	O	GLU	A	255	24.057	7.246	11.708	1.00	12.64
ATOM	1629	CB	GLU	A	255	23.070	10.171	12.468	1.00	11.82
ATOM	1630	CG	GLU	A	255	24.429	9.969	13.135	1.00	9.96
ATOM	1631	CD	GLU	A	255	24.688	10.952	14.267	1.00	11.66
ATOM	1632	OE1	GLU	A	255	23.835	11.819	14.516	1.00	16.47
ATOM	1633	OE2	GLU	A	255	25.749	10.860	14.906	1.00	15.14
ATOM	1634	N	MET	A	256	21.832	7.181	11.966	1.00	12.10
ATOM	1635	CA	MET	A	256	21.807	5.758	12.330	1.00	14.61
ATOM	1636	C	MET	A	256	22.287	4.926	11.108	1.00	16.74
ATOM	1637	O	MET	A	256	23.138	4.052	11.240	1.00	21.09
ATOM	1638	CB	MET	A	256	20.387	5.342	12.784	1.00	12.40
ATOM	1639	CG	MET	A	256	20.029	5.634	14.253	1.00	12.89
ATOM	1640	SD	MET	A	256	18.257	5.851	14.578	1.00	23.36
ATOM	1641	CE	MET	A	256	18.048	5.009	16.025	1.00	16.21
ATOM	1642	N	VAL	A	257	21.816	5.282	9.916	1.00	17.44
ATOM	1643	CA	VAL	A	257	22.184	4.599	8.674	1.00	18.71
ATOM	1644	C	VAL	A	257	23.534	5.043	8.106	1.00	20.14
ATOM	1645	O	VAL	A	257	24.335	4.213	7.690	1.00	23.29
ATOM	1646	CB	VAL	A	257	21.108	4.787	7.540	1.00	19.20
ATOM	1647	CG1	VAL	A	257	19.684	4.702	8.093	1.00	14.26
ATOM	1648	CG2	VAL	A	257	21.304	6.110	6.822	1.00	21.30
ATOM	1649	N	ARG	A	258	23.808	6.343	8.102	1.00	19.80

FIG. 2CC

ATOM	1650	CA	ARG	A	258	25.057	6.854	7.559	1.00	19.39
ATOM	1651	C	ARG	A	258	26.292	6.724	8.448	1.00	22.54
ATOM	1652	O	ARG	A	258	27.426	6.741	7.952	1.00	25.87
ATOM	1653	CB	ARG	A	258	24.880	8.314	7.149	1.00	19.45
ATOM	1654	CG	ARG	A	258	26.141	8.897	6.558	1.00	21.22
ATOM	1655	CD	ARG	A	258	26.013	10.368	6.322	1.00	24.45
ATOM	1656	NE	ARG	A	258	25.130	10.640	5.202	1.00	28.85
ATOM	1657	CZ	ARG	A	258	25.013	11.829	4.629	1.00	30.35
ATOM	1658	NH1	ARG	A	258	25.737	12.844	5.097	1.00	33.58
ATOM	1659	NH2	ARG	A	258	24.192	12.005	3.591	1.00	26.26
ATOM	1660	N	HIS	A	259	26.068	6.557	9.750	1.00	25.71
ATOM	1661	CA	HIS	A	259	27.118	6.449	10.785	1.00	27.73
ATOM	1662	C	HIS	A	259	28.103	7.621	10.883	1.00	28.00
ATOM	1663	O	HIS	A	259	29.309	7.469	11.103	1.00	29.52
ATOM	1664	CB	HIS	A	259	27.805	5.055	10.818	1.00	26.36
ATOM	1665	CG	HIS	A	259	26.879	3.943	11.229	1.00	22.98
ATOM	1666	ND1	HIS	A	259	26.446	3.763	12.527	1.00	22.41
ATOM	1667	CD2	HIS	A	259	26.213	3.021	10.492	1.00	20.61
ATOM	1668	CE1	HIS	A	259	25.549	2.795	12.566	1.00	19.01
ATOM	1669	NE2	HIS	A	259	25.387	2.329	11.347	1.00	16.47
ATOM	1670	N	LYS	A	260	27.539	8.801	10.696	1.00	29.63
ATOM	1671	CA	LYS	A	260	28.243	10.066	10.819	1.00	30.40
ATOM	1672	C	LYS	A	260	27.206	11.193	10.863	1.00	26.07
ATOM	1673	O	LYS	A	260	26.077	11.041	10.380	1.00	24.49
ATOM	1674	CB	LYS	A	260	29.291	10.267	9.721	1.00	33.87
ATOM	1675	CG	LYS	A	260	30.720	10.237	10.297	1.00	40.62
ATOM	1676	CD	LYS	A	260	30.871	11.271	11.428	1.00	46.13
ATOM	1677	CE	LYS	A	260	31.363	10.641	12.733	1.00	48.31
ATOM	1678	NZ	LYS	A	260	30.799	11.393	13.894	1.00	47.46
ATOM	1679	N	ILE	A	261	27.532	12.283	11.542	1.00	22.60
ATOM	1680	CA	ILE	A	261	26.578	13.381	11.642	1.00	19.96
ATOM	1681	C	ILE	A	261	26.353	14.027	10.272	1.00	17.51
ATOM	1682	O	ILE	A	261	27.286	14.420	9.585	1.00	17.46
ATOM	1683	CB	ILE	A	261	27.007	14.436	12.719	1.00	18.47
ATOM	1684	CG1	ILE	A	261	27.110	13.771	14.090	1.00	15.26
ATOM	1685	CG2	ILE	A	261	25.959	15.561	12.833	1.00	20.19
ATOM	1686	CD1	ILE	A	261	28.022	14.488	15.024	1.00	19.17
ATOM	1687	N	LEU	A	262	25.095	14.045	9.871	1.00	17.50
ATOM	1688	CA	LEU	A	262	24.659	14.617	8.607	1.00	18.94
ATOM	1689	C	LEU	A	262	25.138	16.066	8.372	1.00	20.67
ATOM	1690	O	LEU	A	262	25.938	16.328	7.466	1.00	22.13
ATOM	1691	CB	LEU	A	262	23.128	14.559	8.550	1.00	13.08
ATOM	1692	CG	LEU	A	262	22.423	13.385	7.868	1.00	14.46
ATOM	1693	CD1	LEU	A	262	22.952	12.062	8.369	1.00	14.89
ATOM	1694	CD2	LEU	A	262	20.942	13.488	8.066	1.00	7.56
ATOM	1695	N	PHE	A	263	24.702	16.986	9.226	1.00	20.64
ATOM	1696	CA	PHE	A	263	25.034	18.397	9.069	1.00	20.07
ATOM	1697	C	PHE	A	263	25.969	18.969	10.151	1.00	20.50
ATOM	1698	O	PHE	A	263	25.579	19.819	10.959	1.00	20.92
ATOM	1699	CB	PHE	A	263	23.719	19.193	8.998	1.00	18.23
ATOM	1700	CG	PHE	A	263	22.697	18.609	8.022	1.00	14.68
ATOM	1701	CD1	PHE	A	263	22.953	18.563	6.653	1.00	12.98
ATOM	1702	CD2	PHE	A	263	21.484	18.118	8.473	1.00	9.26
ATOM	1703	CE1	PHE	A	263	22.016	18.029	5.760	1.00	8.44
ATOM	1704	CE2	PHE	A	263	20.551	17.586	7.584	1.00	5.41
ATOM	1705	CZ	PHE	A	263	20.824	17.541	6.222	1.00	3.79
ATOM	1706	N	PRO	A	264	27.229	18.528	10.159	1.00	19.70
ATOM	1707	CA	PRO	A	264	28.184	19.012	11.160	1.00	23.64
ATOM	1708	C	PRO	A	264	28.643	20.436	10.950	1.00	25.18

FIG. 2DD

ATOM	1709	O	PRO	A	264	28.040	21.173	10.185	1.00	25.01
ATOM	1710	CB	PRO	A	264	29.339	18.026	11.024	1.00	22.88
ATOM	1711	CG	PRO	A	264	29.272	17.638	9.570	1.00	20.00
ATOM	1712	CD	PRO	A	264	27.814	17.464	9.341	1.00	19.45
ATOM	1713	N	GLY	A	265	29.741	20.807	11.606	1.00	27.92
ATOM	1714	CA	GLY	A	265	30.254	22.160	11.447	1.00	32.00
ATOM	1715	C	GLY	A	265	31.038	22.802	12.586	1.00	32.60
ATOM	1716	O	GLY	A	265	32.079	22.306	13.047	1.00	33.24
ATOM	1717	N	ARG	A	266	30.571	23.976	12.985	1.00	31.55
ATOM	1718	CA	ARG	A	266	31.197	24.726	14.058	1.00	32.94
ATOM	1719	C	ARG	A	266	30.200	25.778	14.485	1.00	33.00
ATOM	1720	O	ARG	A	266	30.019	26.043	15.670	1.00	31.47
ATOM	1721	CB	ARG	A	266	32.486	25.401	13.576	1.00	34.09
ATOM	1722	CG	ARG	A	266	32.327	26.393	12.414	1.00	33.36
ATOM	1723	CD	ARG	A	266	33.694	26.964	12.003	1.00	31.74
ATOM	1724	NE	ARG	A	266	33.653	27.527	10.659	1.00	30.39
ATOM	1725	CZ	ARG	A	266	34.718	27.748	9.900	1.00	24.25
ATOM	1726	NH1	ARG	A	266	35.935	27.483	10.346	1.00	25.66
ATOM	1727	NH2	ARG	A	266	34.552	28.132	8.648	1.00	25.54
ATOM	1728	N	ASP	A	267	29.513	26.327	13.491	1.00	33.80
ATOM	1729	CA	ASP	A	267	28.532	27.358	13.714	1.00	30.50
ATOM	1730	C	ASP	A	267	27.459	27.230	12.656	1.00	26.92
ATOM	1731	O	ASP	A	267	27.676	26.614	11.627	1.00	26.99
ATOM	1732	CB	ASP	A	267	29.198	28.723	13.611	1.00	37.49
ATOM	1733	CG	ASP	A	267	28.284	29.820	14.030	1.00	40.83
ATOM	1734	OD1	ASP	A	267	27.949	30.663	13.175	1.00	44.75
ATOM	1735	OD2	ASP	A	267	27.844	29.799	15.202	1.00	44.89
ATOM	1736	N	TYR	A	268	26.330	27.875	12.907	1.00	25.13
ATOM	1737	CA	TYR	A	268	25.173	27.877	12.030	1.00	24.71
ATOM	1738	C	TYR	A	268	25.444	28.208	10.557	1.00	25.16
ATOM	1739	O	TYR	A	268	24.569	28.030	9.715	1.00	26.18
ATOM	1740	CB	TYR	A	268	24.173	28.889	12.551	1.00	23.88
ATOM	1741	CG	TYR	A	268	23.318	28.454	13.701	1.00	25.55
ATOM	1742	CD1	TYR	A	268	23.505	27.243	14.348	1.00	24.78
ATOM	1743	CD2	TYR	A	268	22.257	29.242	14.100	1.00	28.07
ATOM	1744	CE1	TYR	A	268	22.629	26.834	15.367	1.00	26.43
ATOM	1745	CE2	TYR	A	268	21.395	28.852	15.101	1.00	29.67
ATOM	1746	CZ	TYR	A	268	21.576	27.652	15.734	1.00	28.32
ATOM	1747	OH	TYR	A	268	20.679	27.306	16.720	1.00	30.67
ATOM	1748	N	ILE	A	269	26.610	28.772	10.261	1.00	25.39
ATOM	1749	CA	ILE	A	269	26.971	29.136	8.891	1.00	24.88
ATOM	1750	C	ILE	A	269	27.425	27.850	8.230	1.00	24.23
ATOM	1751	O	ILE	A	269	26.853	27.412	7.235	1.00	23.59
ATOM	1752	CB	ILE	A	269	28.196	30.118	8.842	1.00	24.89
ATOM	1753	CG1	ILE	A	269	27.904	31.463	9.519	1.00	24.46
ATOM	1754	CG2	ILE	A	269	28.638	30.324	7.411	1.00	25.64
ATOM	1755	CD1	ILE	A	269	26.977	32.369	8.767	1.00	21.32
ATOM	1756	N	ASP	A	270	28.468	27.268	8.823	1.00	24.17
ATOM	1757	CA	ASP	A	270	29.099	26.020	8.374	1.00	26.59
ATOM	1758	C	ASP	A	270	28.009	24.978	8.119	1.00	26.04
ATOM	1759	O	ASP	A	270	27.804	24.492	7.003	1.00	26.38
ATOM	1760	CB	ASP	A	270	30.058	25.526	9.483	1.00	25.96
ATOM	1761	CG	ASP	A	270	31.198	24.667	8.959	1.00	23.06
ATOM	1762	OD1	ASP	A	270	32.246	24.588	9.624	1.00	19.74
ATOM	1763	OD2	ASP	A	270	31.055	24.060	7.880	1.00	31.30
ATOM	1764	N	GLN	A	271	27.234	24.764	9.168	1.00	25.91
ATOM	1765	CA	GLN	A	271	26.133	23.820	9.211	1.00	24.57
ATOM	1766	C	GLN	A	271	25.089	24.056	8.121	1.00	23.81
ATOM	1767	O	GLN	A	271	24.563	23.103	7.549	1.00	25.98

FIG. 2EE

ATOM	1768	CB	GLN	A	271	25.501	23.926	10.593	1.00	25.83
ATOM	1769	CG	GLN	A	271	24.574	22.818	10.984	1.00	27.68
ATOM	1770	CD	GLN	A	271	24.013	23.050	12.357	1.00	26.89
ATOM	1771	OE1	GLN	A	271	24.725	23.485	13.281	1.00	23.91
ATOM	1772	NE2	GLN	A	271	22.726	22.781	12.504	1.00	25.73
ATOM	1773	N	TRP	A	272	24.763	25.311	7.830	1.00	22.13
ATOM	1774	CA	TRP	A	272	23.783	25.576	6.788	1.00	19.21
ATOM	1775	C	TRP	A	272	24.419	25.204	5.457	1.00	18.17
ATOM	1776	O	TRP	A	272	23.751	24.749	4.534	1.00	16.56
ATOM	1777	CB	TRP	A	272	23.358	27.037	6.775	1.00	17.37
ATOM	1778	CG	TRP	A	272	22.364	27.377	5.686	1.00	13.75
ATOM	1779	CD1	TRP	A	272	22.557	28.269	4.659	1.00	15.40
ATOM	1780	CD2	TRP	A	272	21.006	26.884	5.535	1.00	15.21
ATOM	1781	NE1	TRP	A	272	21.412	28.374	3.897	1.00	16.90
ATOM	1782	CE2	TRP	A	272	20.446	27.542	4.408	1.00	14.39
ATOM	1783	CE3	TRP	A	272	20.217	25.965	6.241	1.00	14.65
ATOM	1784	CZ2	TRP	A	272	19.130	27.298	3.971	1.00	14.28
ATOM	1785	CZ3	TRP	A	272	18.909	25.725	5.808	1.00	13.40
ATOM	1786	CH2	TRP	A	272	18.377	26.391	4.686	1.00	16.96
ATOM	1787	N	ASN	A	273	25.729	25.353	5.377	1.00	19.02
ATOM	1788	CA	ASN	A	273	26.408	25.013	4.146	1.00	22.48
ATOM	1789	C	ASN	A	273	26.158	23.544	3.866	1.00	22.47
ATOM	1790	O	ASN	A	273	25.748	23.187	2.759	1.00	22.01
ATOM	1791	CB	ASN	A	273	27.912	25.316	4.238	1.00	22.52
ATOM	1792	CG	ASN	A	273	28.227	26.798	4.062	1.00	21.44
ATOM	1793	OD1	ASN	A	273	27.348	27.621	3.781	1.00	21.70
ATOM	1794	ND2	ASN	A	273	29.488	27.143	4.209	1.00	24.93
ATOM	1795	N	LYS	A	274	26.278	22.719	4.914	1.00	23.46
ATOM	1796	CA	LYS	A	274	26.072	21.271	4.805	1.00	18.10
ATOM	1797	C	LYS	A	274	24.626	20.942	4.475	1.00	18.00
ATOM	1798	O	LYS	A	274	24.361	19.937	3.833	1.00	22.35
ATOM	1799	CB	LYS	A	274	26.451	20.566	6.093	1.00	15.27
ATOM	1800	CG	LYS	A	274	27.811	20.904	6.600	1.00	14.30
ATOM	1801	CD	LYS	A	274	28.900	20.434	5.691	1.00	19.69
ATOM	1802	CE	LYS	A	274	30.186	20.267	6.502	1.00	24.70
ATOM	1803	NZ	LYS	A	274	31.204	19.327	5.896	1.00	31.99
ATOM	1804	N	VAL	A	275	23.680	21.770	4.898	1.00	18.18
ATOM	1805	CA	VAL	A	275	22.286	21.487	4.581	1.00	20.59
ATOM	1806	C	VAL	A	275	21.968	21.762	3.110	1.00	23.32
ATOM	1807	O	VAL	A	275	21.204	21.023	2.486	1.00	25.67
ATOM	1808	CB	VAL	A	275	21.282	22.310	5.449	1.00	17.97
ATOM	1809	CG1	VAL	A	275	19.836	21.995	5.045	1.00	15.19
ATOM	1810	CG2	VAL	A	275	21.498	22.025	6.928	1.00	19.77
ATOM	1811	N	ILE	A	276	22.580	22.801	2.547	1.00	23.82
ATOM	1812	CA	ILE	A	276	22.320	23.168	1.164	1.00	20.92
ATOM	1813	C	ILE	A	276	23.120	22.356	0.147	1.00	20.60
ATOM	1814	O	ILE	A	276	22.640	22.087	-0.952	1.00	23.64
ATOM	1815	CB	ILE	A	276	22.506	24.703	0.926	1.00	18.18
ATOM	1816	CG1	ILE	A	276	23.916	25.139	1.336	1.00	18.15
ATOM	1817	CG2	ILE	A	276	21.429	25.464	1.643	1.00	9.12
ATOM	1818	CD1	ILE	A	276	24.426	26.400	0.674	1.00	16.28
ATOM	1819	N	GLU	A	277	24.313	21.923	0.511	1.00	20.50
ATOM	1820	CA	GLU	A	277	25.091	21.156	-0.423	1.00	23.41
ATOM	1821	C	GLU	A	277	24.653	19.705	-0.550	1.00	28.35
ATOM	1822	O	GLU	A	277	25.080	19.002	-1.468	1.00	34.25
ATOM	1823	CB	GLU	A	277	26.572	21.265	-0.117	1.00	19.67
ATOM	1824	CG	GLU	A	277	27.058	20.421	0.982	1.00	24.35
ATOM	1825	CD	GLU	A	277	28.553	20.552	1.136	1.00	30.31
ATOM	1826	OE1	GLU	A	277	29.232	19.510	1.313	1.00	35.18

FIG. 2FF

ATOM	1827	OE2	GLU	A	277	29.050	21.704	1.058	1.00	28.91
ATOM	1828	N	GLN	A	278	23.795	19.245	0.350	1.00	26.32
ATOM	1829	CA	GLN	A	278	23.316	17.880	0.283	1.00	22.89
ATOM	1830	C	GLN	A	278	21.888	17.806	-0.235	1.00	22.44
ATOM	1831	O	GLN	A	278	21.580	16.978	-1.089	1.00	23.76
ATOM	1832	CB	GLN	A	278	23.422	17.212	1.649	1.00	23.63
ATOM	1833	CG	GLN	A	278	24.850	17.022	2.111	1.00	25.91
ATOM	1834	CD	GLN	A	278	24.918	16.301	3.446	1.00	29.41
ATOM	1835	OE1	GLN	A	278	24.521	15.139	3.552	1.00	26.75
ATOM	1836	NE2	GLN	A	278	25.407	16.993	4.476	1.00	30.71
ATOM	1837	N	LEU	A	279	21.018	18.676	0.263	1.00	20.12
ATOM	1838	CA	LEU	A	279	19.628	18.681	-0.171	1.00	20.56
ATOM	1839	C	LEU	A	279	19.369	19.804	-1.200	1.00	20.66
ATOM	1840	O	LEU	A	279	18.273	19.908	-1.758	1.00	20.40
ATOM	1841	CB	LEU	A	279	18.678	18.852	1.036	1.00	19.86
ATOM	1842	CG	LEU	A	279	18.904	18.176	2.405	1.00	19.25
ATOM	1843	CD1	LEU	A	279	17.786	18.595	3.383	1.00	12.82
ATOM	1844	CD2	LEU	A	279	18.967	16.661	2.278	1.00	17.53
ATOM	1845	N	GLY	A	280	20.365	20.663	-1.402	1.00	21.53
ATOM	1846	CA	GLY	A	280	20.243	21.768	-2.338	1.00	21.98
ATOM	1847	C	GLY	A	280	19.735	23.072	-1.749	1.00	24.54
ATOM	1848	O	GLY	A	280	19.401	23.165	-0.569	1.00	26.75
ATOM	1849	N	THR	A	281	19.648	24.095	-2.585	1.00	24.49
ATOM	1850	CA	THR	A	281	19.174	25.394	-2.145	1.00	28.73
ATOM	1851	C	THR	A	281	17.633	25.347	-2.013	1.00	30.15
ATOM	1852	O	THR	A	281	16.956	24.708	-2.818	1.00	31.24
ATOM	1853	CB	THR	A	281	19.675	26.539	-3.129	1.00	30.04
ATOM	1854	OG1	THR	A	281	21.040	26.284	-3.514	1.00	29.30
ATOM	1855	CG2	THR	A	281	19.649	27.912	-2.450	1.00	31.80
ATOM	1856	N	PRO	A	282	17.074	25.969	-0.951	1.00	30.63
ATOM	1857	CA	PRO	A	282	15.621	25.973	-0.742	1.00	31.39
ATOM	1858	C	PRO	A	282	14.790	26.593	-1.860	1.00	35.04
ATOM	1859	O	PRO	A	282	15.137	27.622	-2.442	1.00	34.15
ATOM	1860	CB	PRO	A	282	15.465	26.736	0.576	1.00	27.71
ATOM	1861	CG	PRO	A	282	16.711	26.411	1.309	1.00	28.19
ATOM	1862	CD	PRO	A	282	17.763	26.542	0.215	1.00	26.87
ATOM	1863	N	CYS	A	283	13.651	25.954	-2.102	1.00	39.56
ATOM	1864	CA	CYS	A	283	12.678	26.348	-3.116	1.00	42.11
ATOM	1865	C	CYS	A	283	12.300	27.819	-3.079	1.00	41.47
ATOM	1866	O	CYS	A	283	12.033	28.363	-2.022	1.00	39.65
ATOM	1867	CB	CYS	A	283	11.401	25.508	-2.936	1.00	45.67
ATOM	1868	SG	CYS	A	283	10.669	25.546	-1.228	1.00	49.59
ATOM	1869	N	PRO	A	284	12.415	28.507	-4.220	1.00	43.20
ATOM	1870	CA	PRO	A	284	12.071	29.933	-4.341	1.00	43.55
ATOM	1871	C	PRO	A	284	10.618	30.191	-3.925	1.00	43.04
ATOM	1872	O	PRO	A	284	9.676	30.140	-4.735	1.00	43.04
ATOM	1873	CB	PRO	A	284	12.321	30.241	-5.826	1.00	44.13
ATOM	1874	CG	PRO	A	284	12.722	28.883	-6.460	1.00	47.78
ATOM	1875	CD	PRO	A	284	13.306	28.106	-5.318	1.00	44.72
ATOM	1876	N	ALA	A	285	10.471	30.388	-2.619	1.00	40.82
ATOM	1877	CA	ALA	A	285	9.196	30.634	-1.951	1.00	39.42
ATOM	1878	C	ALA	A	285	9.559	30.601	-0.465	1.00	39.31
ATOM	1879	O	ALA	A	285	9.146	31.462	0.307	1.00	41.09
ATOM	1880	CB	ALA	A	285	8.193	29.514	-2.275	1.00	39.41
ATOM	1881	N	PHE	A	286	10.356	29.591	-0.096	1.00	36.13
ATOM	1882	CA	PHE	A	286	10.840	29.373	1.261	1.00	29.31
ATOM	1883	C	PHE	A	286	11.473	30.642	1.819	1.00	29.93
ATOM	1884	O	PHE	A	286	11.137	31.087	2.923	1.00	27.02
ATOM	1885	CB	PHE	A	286	11.869	28.251	1.237	1.00	25.30

FIG. 2GG

ATOM	1886	CG	PHE	A	286	12.446	27.931	2.581	1.00	18.21
ATOM	1887	CD1	PHE	A	286	11.621	27.534	3.624	1.00	18.09
ATOM	1888	CD2	PHE	A	286	13.811	28.035	2.805	1.00	15.83
ATOM	1889	CE1	PHE	A	286	12.154	27.245	4.887	1.00	18.38
ATOM	1890	CE2	PHE	A	286	14.357	27.754	4.052	1.00	18.25
ATOM	1891	CZ	PHE	A	286	13.533	27.357	5.097	1.00	15.03
ATOM	1892	N	MET	A	287	12.340	31.256	1.019	1.00	32.98
ATOM	1893	CA	MET	A	287	13.021	32.485	1.411	1.00	35.50
ATOM	1894	C	MET	A	287	12.110	33.659	1.797	1.00	35.57
ATOM	1895	O	MET	A	287	12.566	34.586	2.456	1.00	36.21
ATOM	1896	CB	MET	A	287	13.986	32.935	0.312	1.00	37.48
ATOM	1897	CG	MET	A	287	15.377	32.320	0.388	1.00	38.29
ATOM	1898	SD	MET	A	287	15.506	30.652	-0.248	1.00	42.69
ATOM	1899	CE	MET	A	287	15.218	30.918	-1.938	1.00	39.17
ATOM	1900	N	LYS	A	288	10.833	33.607	1.428	1.00	36.32
ATOM	1901	CA	LYS	A	288	9.895	34.678	1.753	1.00	37.98
ATOM	1902	C	LYS	A	288	9.604	34.812	3.251	1.00	41.25
ATOM	1903	O	LYS	A	288	9.347	35.919	3.748	1.00	42.92
ATOM	1904	CB	LYS	A	288	8.573	34.480	1.004	1.00	39.11
ATOM	1905	CG	LYS	A	288	8.479	35.161	-0.371	1.00	42.11
ATOM	1906	CD	LYS	A	288	9.372	34.565	-1.463	1.00	44.65
ATOM	1907	CE	LYS	A	288	9.066	35.248	-2.815	1.00	47.02
ATOM	1908	NZ	LYS	A	288	9.881	34.775	-3.985	1.00	45.67
ATOM	1909	N	LYS	A	289	9.611	33.691	3.969	1.00	41.56
ATOM	1910	CA	LYS	A	289	9.345	33.722	5.407	1.00	40.78
ATOM	1911	C	LYS	A	289	10.626	33.990	6.206	1.00	39.17
ATOM	1912	O	LYS	A	289	10.643	33.955	7.452	1.00	38.50
ATOM	1913	CB	LYS	A	289	8.692	32.415	5.850	1.00	43.27
ATOM	1914	CG	LYS	A	289	7.262	32.219	5.330	1.00	47.51
ATOM	1915	CD	LYS	A	289	6.305	33.345	5.782	1.00	51.55
ATOM	1916	CE	LYS	A	289	6.180	33.475	7.313	1.00	52.02
ATOM	1917	NZ	LYS	A	289	7.275	34.267	7.960	1.00	54.69
ATOM	1918	N	LEU	A	290	11.670	34.336	5.462	1.00	36.37
ATOM	1919	CA	LEU	A	290	12.992	34.622	6.001	1.00	36.82
ATOM	1920	C	LEU	A	290	13.167	36.136	6.198	1.00	37.74
ATOM	1921	O	LEU	A	290	13.092	36.896	5.227	1.00	39.91
ATOM	1922	CB	LEU	A	290	14.013	34.103	4.993	1.00	32.06
ATOM	1923	CG	LEU	A	290	15.236	33.276	5.380	1.00	32.32
ATOM	1924	CD1	LEU	A	290	15.046	32.512	6.675	1.00	28.02
ATOM	1925	CD2	LEU	A	290	15.564	32.341	4.224	1.00	27.96
ATOM	1926	N	GLN	A	291	13.399	36.583	7.438	1.00	39.04
ATOM	1927	CA	GLN	A	291	13.584	38.021	7.711	1.00	38.20
ATOM	1928	C	GLN	A	291	14.561	38.548	6.664	1.00	37.52
ATOM	1929	O	GLN	A	291	15.495	37.839	6.267	1.00	36.29
ATOM	1930	CB	GLN	A	291	14.142	38.280	9.123	1.00	39.70
ATOM	1931	CG	GLN	A	291	14.008	39.737	9.641	1.00	43.34
ATOM	1932	CD	GLN	A	291	12.729	39.981	10.459	1.00	43.23
ATOM	1933	OE1	GLN	A	291	12.426	39.218	11.375	1.00	45.26
ATOM	1934	NE2	GLN	A	291	11.989	41.051	10.137	1.00	40.70
ATOM	1935	N	PRO	A	292	14.339	39.787	6.193	1.00	35.64
ATOM	1936	CA	PRO	A	292	15.129	40.485	5.179	1.00	34.65
ATOM	1937	C	PRO	A	292	16.634	40.338	5.292	1.00	35.33
ATOM	1938	O	PRO	A	292	17.325	40.156	4.287	1.00	33.35
ATOM	1939	CB	PRO	A	292	14.665	41.921	5.353	1.00	35.18
ATOM	1940	CG	PRO	A	292	13.221	41.746	5.638	1.00	34.12
ATOM	1941	CD	PRO	A	292	13.282	40.675	6.702	1.00	35.37
ATOM	1942	N	THR	A	293	17.146	40.372	6.510	1.00	37.57
ATOM	1943	CA	THR	A	293	18.585	40.230	6.697	1.00	39.75
ATOM	1944	C	THR	A	293	19.050	38.772	6.627	1.00	39.13

FIG. 2HH

ATOM	1945	O	THR	A	293	20.210	38.506	6.289	1.00	37.75
ATOM	1946	CB	THR	A	293	19.043	40.827	8.035	1.00	42.63
ATOM	1947	OG1	THR	A	293	18.061	41.766	8.512	1.00	47.19
ATOM	1948	CG2	THR	A	293	20.419	41.515	7.852	1.00	40.06
ATOM	1949	N	VAL	A	294	18.159	37.843	6.988	1.00	36.77
ATOM	1950	CA	VAL	A	294	18.464	36.413	6.956	1.00	34.85
ATOM	1951	C	VAL	A	294	18.343	35.930	5.536	1.00	33.86
ATOM	1952	O	VAL	A	294	19.169	35.154	5.060	1.00	33.38
ATOM	1953	CB	VAL	A	294	17.450	35.566	7.738	1.00	34.91
ATOM	1954	CG1	VAL	A	294	17.953	34.144	7.816	1.00	35.42
ATOM	1955	CG2	VAL	A	294	17.213	36.124	9.127	1.00	37.51
ATOM	1956	N	ARG	A	295	17.297	36.404	4.867	1.00	33.96
ATOM	1957	CA	ARG	A	295	17.020	36.035	3.492	1.00	34.52
ATOM	1958	C	ARG	A	295	18.099	36.552	2.544	1.00	36.07
ATOM	1959	O	ARG	A	295	18.361	35.940	1.502	1.00	37.40
ATOM	1960	CB	ARG	A	295	15.636	36.534	3.070	1.00	34.81
ATOM	1961	CG	ARG	A	295	15.619	37.953	2.559	1.00	36.10
ATOM	1962	CD	ARG	A	295	14.402	38.189	1.706	1.00	30.72
ATOM	1963	NE	ARG	A	295	13.204	38.284	2.511	1.00	26.85
ATOM	1964	CZ	ARG	A	295	11.981	38.371	2.008	1.00	30.88
ATOM	1965	NH1	ARG	A	295	11.790	38.366	0.694	1.00	33.56
ATOM	1966	NH2	ARG	A	295	10.946	38.518	2.822	1.00	34.68
ATOM	1967	N	ASN	A	296	18.736	37.666	2.899	1.00	35.96
ATOM	1968	CA	ASN	A	296	19.790	38.224	2.072	1.00	33.95
ATOM	1969	C	ASN	A	296	20.923	37.225	1.996	1.00	33.60
ATOM	1970	O	ASN	A	296	21.366	36.868	0.899	1.00	34.00
ATOM	1971	CB	ASN	A	296	20.333	39.510	2.680	1.00	36.06
ATOM	1972	CG	ASN	A	296	21.513	40.050	1.906	1.00	35.72
ATOM	1973	OD1	ASN	A	296	21.331	40.659	0.858	1.00	36.39
ATOM	1974	ND2	ASN	A	296	22.732	39.772	2.381	1.00	34.76
ATOM	1975	N	TYR	A	297	21.408	36.802	3.172	1.00	31.97
ATOM	1976	CA	TYR	A	297	22.498	35.819	3.309	1.00	29.60
ATOM	1977	C	TYR	A	297	22.218	34.521	2.549	1.00	28.11
ATOM	1978	O	TYR	A	297	23.084	34.020	1.840	1.00	28.70
ATOM	1979	CB	TYR	A	297	22.740	35.481	4.795	1.00	26.28
ATOM	1980	CG	TYR	A	297	23.722	34.341	5.021	1.00	26.96
ATOM	1981	CD1	TYR	A	297	25.091	34.533	4.887	1.00	25.56
ATOM	1982	CD2	TYR	A	297	23.277	33.061	5.346	1.00	27.53
ATOM	1983	CE1	TYR	A	297	25.986	33.486	5.061	1.00	25.70
ATOM	1984	CE2	TYR	A	297	24.169	32.012	5.518	1.00	26.17
ATOM	1985	CZ	TYR	A	297	25.520	32.229	5.367	1.00	25.43
ATOM	1986	OH	TYR	A	297	26.406	31.179	5.452	1.00	28.49
ATOM	1987	N	VAL	A	298	21.006	33.996	2.711	1.00	28.24
ATOM	1988	CA	VAL	A	298	20.569	32.750	2.102	1.00	27.73
ATOM	1989	C	VAL	A	298	20.413	32.855	0.589	1.00	29.27
ATOM	1990	O	VAL	A	298	20.990	32.055	-0.158	1.00	28.77
ATOM	1991	CB	VAL	A	298	19.238	32.288	2.758	1.00	26.32
ATOM	1992	CG1	VAL	A	298	18.614	31.158	1.992	1.00	29.24
ATOM	1993	CG2	VAL	A	298	19.490	31.872	4.209	1.00	29.06
ATOM	1994	N	GLU	A	299	19.687	33.876	0.131	1.00	30.27
ATOM	1995	CA	GLU	A	299	19.452	34.088	-1.295	1.00	28.19
ATOM	1996	C	GLU	A	299	20.767	34.320	-1.981	1.00	27.95
ATOM	1997	O	GLU	A	299	20.897	34.065	-3.171	1.00	29.01
ATOM	1998	CB	GLU	A	299	18.562	35.302	-1.539	1.00	28.56
ATOM	1999	CG	GLU	A	299	17.151	35.179	-0.992	1.00	32.18
ATOM	2000	CD	GLU	A	299	16.093	35.665	-1.971	1.00	36.34
ATOM	2001	OE1	GLU	A	299	14.993	36.076	-1.516	1.00	37.16
ATOM	2002	OE2	GLU	A	299	16.356	35.604	-3.199	1.00	37.87
ATOM	2003	N	ASN	A	300	21.746	34.799	-1.218	1.00	29.48

FIG. 2II

ATOM	2004	CA	ASN	A	300	23.067	35.083	-1.747	1.00	27.96
ATOM	2005	C	ASN	A	300	24.104	34.004	-1.491	1.00	26.74
ATOM	2006	O	ASN	A	300	25.291	34.304	-1.451	1.00	27.37
ATOM	2007	CB	ASN	A	300	23.581	36.412	-1.191	1.00	32.01
ATOM	2008	CG	ASN	A	300	22.759	37.609	-1.649	1.00	34.99
ATOM	2009	OD1	ASN	A	300	22.608	38.572	-0.908	1.00	40.39
ATOM	2010	ND2	ASN	A	300	22.236	37.560	-2.874	1.00	40.11
ATOM	2011	N	ARG	A	301	23.675	32.754	-1.323	1.00	29.11
ATOM	2012	CA	ARG	A	301	24.618	31.646	-1.070	1.00	29.04
ATOM	2013	C	ARG	A	301	24.922	30.886	-2.369	1.00	28.33
ATOM	2014	O	ARG	A	301	24.077	30.856	-3.272	1.00	25.54
ATOM	2015	CB	ARG	A	301	24.026	30.593	-0.083	1.00	25.95
ATOM	2016	CG	ARG	A	301	23.797	31.018	1.342	1.00	21.29
ATOM	2017	CD	ARG	A	301	25.069	31.501	1.958	1.00	20.39
ATOM	2018	NE	ARG	A	301	26.164	30.562	1.784	1.00	20.66
ATOM	2019	CZ	ARG	A	301	27.443	30.867	1.989	1.00	26.05
ATOM	2020	NH1	ARG	A	301	27.775	32.094	2.365	1.00	29.37
ATOM	2021	NH2	ARG	A	301	28.397	29.946	1.873	1.00	27.83
ATOM	2022	N	PRO	A	302	26.152	30.314	-2.489	1.00	29.03
ATOM	2023	CA	PRO	A	302	26.561	29.535	-3.668	1.00	31.83
ATOM	2024	C	PRO	A	302	25.470	28.465	-3.932	1.00	34.72
ATOM	2025	O	PRO	A	302	25.181	27.637	-3.054	1.00	36.10
ATOM	2026	CB	PRO	A	302	27.894	28.877	-3.225	1.00	29.18
ATOM	2027	CG	PRO	A	302	28.211	29.449	-1.841	1.00	27.99
ATOM	2028	CD	PRO	A	302	27.323	30.659	-1.666	1.00	27.00
ATOM	2029	N	ALA	A	303	24.825	28.519	-5.100	1.00	35.33
ATOM	2030	CA	ALA	A	303	23.756	27.574	-5.425	1.00	32.36
ATOM	2031	C	ALA	A	303	24.194	26.103	-5.551	1.00	32.18
ATOM	2032	O	ALA	A	303	25.361	25.784	-5.874	1.00	28.91
ATOM	2033	CB	ALA	A	303	22.960	28.038	-6.637	1.00	31.16
ATOM	2034	N	TYR	A	304	23.245	25.230	-5.188	1.00	33.00
ATOM	2035	CA	TYR	A	304	23.394	23.765	-5.163	1.00	29.61
ATOM	2036	C	TYR	A	304	22.126	23.055	-5.655	1.00	29.37
ATOM	2037	O	TYR	A	304	21.004	23.459	-5.333	1.00	27.81
ATOM	2038	CB	TYR	A	304	23.666	23.284	-3.731	1.00	24.77
ATOM	2039	CG	TYR	A	304	25.116	23.200	-3.363	1.00	24.50
ATOM	2040	CD1	TYR	A	304	25.752	24.240	-2.702	1.00	25.72
ATOM	2041	CD2	TYR	A	304	25.857	22.065	-3.661	1.00	26.30
ATOM	2042	CE1	TYR	A	304	27.095	24.153	-2.345	1.00	29.74
ATOM	2043	CE2	TYR	A	304	27.194	21.962	-3.317	1.00	28.89
ATOM	2044	CZ	TYR	A	304	27.817	23.012	-2.659	1.00	32.70
ATOM	2045	OH	TYR	A	304	29.171	22.939	-2.356	1.00	33.67
ATOM	2046	N	ALA	A	305	22.305	22.025	-6.478	1.00	29.27
ATOM	2047	CA	ALA	A	305	21.167	21.253	-6.968	1.00	28.38
ATOM	2048	C	ALA	A	305	20.752	20.290	-5.867	1.00	26.04
ATOM	2049	O	ALA	A	305	19.581	19.934	-5.738	1.00	23.89
ATOM	2050	CB	ALA	A	305	21.562	20.478	-8.210	1.00	29.32
ATOM	2051	N	GLY	A	306	21.755	19.857	-5.106	1.00	24.87
ATOM	2052	CA	GLY	A	306	21.553	18.937	-4.005	1.00	27.80
ATOM	2053	C	GLY	A	306	21.401	17.523	-4.503	1.00	27.75
ATOM	2054	O	GLY	A	306	20.829	17.320	-5.572	1.00	30.73
ATOM	2055	N	LEU	A	307	21.908	16.546	-3.751	1.00	25.91
ATOM	2056	CA	LEU	A	307	21.812	15.144	-4.162	1.00	22.59
ATOM	2057	C	LEU	A	307	20.478	14.519	-3.831	1.00	23.95
ATOM	2058	O	LEU	A	307	19.732	14.990	-2.958	1.00	24.98
ATOM	2059	CB	LEU	A	307	22.854	14.299	-3.478	1.00	18.77
ATOM	2060	CG	LEU	A	307	24.229	14.866	-3.267	1.00	20.81
ATOM	2061	CD1	LEU	A	307	25.034	13.780	-2.584	1.00	22.83
ATOM	2062	CD2	LEU	A	307	24.864	15.284	-4.571	1.00	23.95

FIG. 2JJ

ATOM	2063	N	THR	A	308	20.179	13.429	-4.529	1.00	24.56
ATOM	2064	CA	THR	A	308	18.945	12.702	-4.269	1.00	22.19
ATOM	2065	C	THR	A	308	19.191	11.838	-3.028	1.00	17.31
ATOM	2066	O	THR	A	308	20.331	11.552	-2.657	1.00	13.75
ATOM	2067	CB	THR	A	308	18.511	11.774	-5.461	1.00	24.54
ATOM	2068	OG1	THR	A	308	19.560	10.851	-5.778	1.00	24.50
ATOM	2069	CG2	THR	A	308	18.121	12.590	-6.681	1.00	21.46
ATOM	2070	N	PHE	A	309	18.111	11.383	-2.425	1.00	17.90
ATOM	2071	CA	PHE	A	309	18.235	10.560	-1.248	1.00	23.22
ATOM	2072	C	PHE	A	309	18.974	9.257	-1.457	1.00	25.08
ATOM	2073	O	PHE	A	309	19.653	8.804	-0.542	1.00	25.85
ATOM	2074	CB	PHE	A	309	16.887	10.374	-0.578	1.00	21.29
ATOM	2075	CG	PHE	A	309	16.452	11.591	0.164	1.00	22.18
ATOM	2076	CD1	PHE	A	309	15.864	12.659	-0.510	1.00	21.34
ATOM	2077	CD2	PHE	A	309	16.736	11.723	1.517	1.00	21.79
ATOM	2078	CE1	PHE	A	309	15.572	13.856	0.158	1.00	22.53
ATOM	2079	CE2	PHE	A	309	16.452	12.909	2.195	1.00	22.27
ATOM	2080	CZ	PHE	A	309	15.866	13.979	1.514	1.00	22.02
ATOM	2081	N	PRO	A	310	18.841	8.625	-2.640	1.00	25.50
ATOM	2082	CA	PRO	A	310	19.543	7.364	-2.888	1.00	22.46
ATOM	2083	C	PRO	A	310	21.041	7.566	-2.970	1.00	22.40
ATOM	2084	O	PRO	A	310	21.806	6.678	-2.613	1.00	24.00
ATOM	2085	CB	PRO	A	310	18.961	6.900	-4.218	1.00	25.65
ATOM	2086	CG	PRO	A	310	17.537	7.358	-4.127	1.00	26.81
ATOM	2087	CD	PRO	A	310	17.721	8.776	-3.602	1.00	27.78
ATOM	2088	N	LYS	A	311	21.468	8.722	-3.459	1.00	26.43
ATOM	2089	CA	LYS	A	311	22.901	9.004	-3.540	1.00	26.72
ATOM	2090	C	LYS	A	311	23.311	9.641	-2.232	1.00	24.76
ATOM	2091	O	LYS	A	311	24.503	9.699	-1.918	1.00	24.86
ATOM	2092	CB	LYS	A	311	23.260	9.885	-4.744	1.00	29.52
ATOM	2093	CG	LYS	A	311	22.367	11.086	-4.950	1.00	32.23
ATOM	2094	CD	LYS	A	311	22.797	11.902	-6.187	1.00	35.53
ATOM	2095	CE	LYS	A	311	22.506	11.184	-7.503	1.00	34.62
ATOM	2096	NZ	LYS	A	311	21.041	11.064	-7.750	1.00	33.92
ATOM	2097	N	LEU	A	312	22.305	10.090	-1.467	1.00	24.19
ATOM	2098	CA	LEU	A	312	22.505	10.685	-0.137	1.00	22.42
ATOM	2099	C	LEU	A	312	22.626	9.531	0.856	1.00	22.08
ATOM	2100	O	LEU	A	312	23.504	9.532	1.724	1.00	22.80
ATOM	2101	CB	LEU	A	312	21.313	11.563	0.253	1.00	18.83
ATOM	2102	CG	LEU	A	312	21.589	13.050	0.097	1.00	15.41
ATOM	2103	CD1	LEU	A	312	20.376	13.839	0.492	1.00	12.74
ATOM	2104	CD2	LEU	A	312	22.791	13.391	0.944	1.00	13.01
ATOM	2105	N	PHE	A	313	21.782	8.521	0.643	1.00	21.73
ATOM	2106	CA	PHE	A	313	21.715	7.305	1.453	1.00	21.11
ATOM	2107	C	PHE	A	313	21.686	6.045	0.565	1.00	21.89
ATOM	2108	O	PHE	A	313	20.628	5.476	0.301	1.00	23.17
ATOM	2109	CB	PHE	A	313	20.477	7.323	2.360	1.00	20.42
ATOM	2110	CG	PHE	A	313	20.457	8.483	3.336	1.00	21.54
ATOM	2111	CD1	PHE	A	313	19.446	9.422	3.281	1.00	21.51
ATOM	2112	CD2	PHE	A	313	21.471	8.645	4.277	1.00	18.24
ATOM	2113	CE1	PHE	A	313	19.451	10.529	4.139	1.00	23.36
ATOM	2114	CE2	PHE	A	313	21.497	9.743	5.144	1.00	20.28
ATOM	2115	CZ	PHE	A	313	20.485	10.687	5.079	1.00	19.77
ATOM	2116	N	PRO	A	314	22.862	5.608	0.104	1.00	22.26
ATOM	2117	CA	PRO	A	314	23.081	4.437	-0.748	1.00	27.78
ATOM	2118	C	PRO	A	314	22.453	3.171	-0.190	1.00	29.90
ATOM	2119	O	PRO	A	314	22.210	3.069	1.006	1.00	29.70
ATOM	2120	CB	PRO	A	314	24.599	4.305	-0.744	1.00	28.60
ATOM	2121	CG	PRO	A	314	25.054	5.722	-0.677	1.00	23.83

FIG. 2KK

ATOM	2122	CD	PRO	A	314	24.138	6.290	0.380	1.00	24.26
ATOM	2123	N	ASP	A	315	22.234	2.190	-1.059	1.00	32.62
ATOM	2124	CA	ASP	A	315	21.627	0.937	-0.641	1.00	35.70
ATOM	2125	C	ASP	A	315	22.591	0.064	0.173	1.00	33.22
ATOM	2126	O	ASP	A	315	22.176	-0.826	0.921	1.00	32.53
ATOM	2127	CB	ASP	A	315	21.080	0.194	-1.864	1.00	41.44
ATOM	2128	CG	ASP	A	315	19.948	-0.767	-1.504	1.00	47.92
ATOM	2129	OD1	ASP	A	315	18.782	-0.303	-1.389	1.00	48.99
ATOM	2130	OD2	ASP	A	315	20.228	-1.986	-1.335	1.00	50.65
ATOM	2131	N	SER	A	316	23.878	0.368	0.041	1.00	32.70
ATOM	2132	CA	SER	A	316	24.945	-0.321	0.753	1.00	32.11
ATOM	2133	C	SER	A	316	24.964	0.046	2.234	1.00	33.20
ATOM	2134	O	SER	A	316	25.765	-0.494	3.008	1.00	33.99
ATOM	2135	CB	SER	A	316	26.296	0.025	0.116	1.00	33.15
ATOM	2136	OG	SER	A	316	26.322	1.361	-0.365	1.00	32.59
ATOM	2137	N	LEU	A	317	24.110	0.996	2.610	1.00	33.53
ATOM	2138	CA	LEU	A	317	23.996	1.446	3.993	1.00	33.28
ATOM	2139	C	LEU	A	317	22.946	0.626	4.721	1.00	35.30
ATOM	2140	O	LEU	A	317	23.066	0.385	5.917	1.00	37.21
ATOM	2141	CB	LEU	A	317	23.603	2.923	4.054	1.00	30.83
ATOM	2142	CG	LEU	A	317	24.645	3.949	3.619	1.00	29.13
ATOM	2143	CD1	LEU	A	317	24.099	5.348	3.856	1.00	26.44
ATOM	2144	CD2	LEU	A	317	25.933	3.718	4.399	1.00	28.48
ATOM	2145	N	PHE	A	318	21.901	0.237	3.999	1.00	36.65
ATOM	2146	CA	PHE	A	318	20.817	-0.550	4.570	1.00	35.98
ATOM	2147	C	PHE	A	318	21.016	-2.003	4.175	1.00	39.10
ATOM	2148	O	PHE	A	318	21.696	-2.303	3.192	1.00	39.40
ATOM	2149	CB	PHE	A	318	19.446	-0.135	4.030	1.00	32.24
ATOM	2150	CG	PHE	A	318	19.156	1.326	4.131	1.00	29.76
ATOM	2151	CD1	PHE	A	318	19.675	2.211	3.192	1.00	30.03
ATOM	2152	CD2	PHE	A	318	18.272	1.800	5.087	1.00	29.55
ATOM	2153	CE1	PHE	A	318	19.320	3.562	3.191	1.00	30.88
ATOM	2154	CE2	PHE	A	318	17.902	3.147	5.107	1.00	32.47
ATOM	2155	CZ	PHE	A	318	18.423	4.038	4.147	1.00	29.56
ATOM	2156	N	PRO	A	319	20.423	-2.923	4.950	1.00	41.02
ATOM	2157	CA	PRO	A	319	20.469	-4.370	4.763	1.00	40.92
ATOM	2158	C	PRO	A	319	19.664	-4.771	3.523	1.00	40.26
ATOM	2159	O	PRO	A	319	18.445	-4.577	3.474	1.00	40.41
ATOM	2160	CB	PRO	A	319	19.817	-4.885	6.046	1.00	40.44
ATOM	2161	CG	PRO	A	319	20.171	-3.830	7.054	1.00	38.98
ATOM	2162	CD	PRO	A	319	19.834	-2.607	6.266	1.00	42.72
ATOM	2163	N	ALA	A	320	20.347	-5.363	2.550	1.00	39.10
ATOM	2164	CA	ALA	A	320	19.712	-5.783	1.315	1.00	39.58
ATOM	2165	C	ALA	A	320	19.866	-7.283	1.086	1.00	39.61
ATOM	2166	O	ALA	A	320	20.040	-7.727	-0.053	1.00	41.72
ATOM	2167	CB	ALA	A	320	20.320	-5.021	0.155	1.00	43.99
ATOM	2168	N	ASP	A	321	19.806	-8.073	2.157	1.00	36.36
ATOM	2169	CA	ASP	A	321	19.962	-9.520	2.026	1.00	31.72
ATOM	2170	C	ASP	A	321	18.675	-10.243	1.709	1.00	29.16
ATOM	2171	O	ASP	A	321	18.680	-11.233	0.980	1.00	33.72
ATOM	2172	CB	ASP	A	321	20.638	-10.134	3.263	1.00	29.58
ATOM	2173	CG	ASP	A	321	20.024	-9.681	4.575	1.00	26.63
ATOM	2174	OD1	ASP	A	321	18.840	-9.279	4.624	1.00	28.64
ATOM	2175	OD2	ASP	A	321	20.757	-9.739	5.573	1.00	27.21
ATOM	2176	N	SER	A	322	17.571	-9.727	2.225	1.00	23.95
ATOM	2177	CA	SER	A	322	16.296	-10.357	1.993	1.00	21.48
ATOM	2178	C	SER	A	322	15.286	-9.388	1.408	1.00	20.22
ATOM	2179	O	SER	A	322	15.500	-8.184	1.384	1.00	20.42
ATOM	2180	CB	SER	A	322	15.763	-10.961	3.295	1.00	25.55

FIG. 2LL

ATOM	2181	OG	SER	A	322	15.116	-9.994	4.117	1.00	29.61
ATOM	2182	N	GLU	A	323	14.168	-9.929	0.955	1.00	18.90
ATOM	2183	CA	GLU	A	323	13.113	-9.134	0.376	1.00	20.38
ATOM	2184	C	GLU	A	323	12.404	-8.299	1.424	1.00	20.46
ATOM	2185	O	GLU	A	323	11.669	-7.373	1.091	1.00	21.68
ATOM	2186	CB	GLU	A	323	12.119	-10.034	-0.349	1.00	17.47
ATOM	2187	CG	GLU	A	323	12.715	-10.719	-1.559	1.00	24.16
ATOM	2188	CD	GLU	A	323	12.708	-9.861	-2.846	1.00	26.03
ATOM	2189	OE1	GLU	A	323	13.040	-10.412	-3.926	1.00	28.72
ATOM	2190	OE2	GLU	A	323	12.358	-8.664	-2.789	1.00	23.50
ATOM	2191	N	HIS	A	324	12.589	-8.638	2.695	1.00	22.03
ATOM	2192	CA	HIS	A	324	11.954	-7.866	3.767	1.00	19.77
ATOM	2193	C	HIS	A	324	12.814	-6.631	4.016	1.00	15.64
ATOM	2194	O	HIS	A	324	12.338	-5.503	3.984	1.00	14.85
ATOM	2195	CB	HIS	A	324	11.832	-8.718	5.041	1.00	18.59
ATOM	2196	CG	HIS	A	324	11.420	-7.938	6.254	1.00	17.00
ATOM	2197	ND1	HIS	A	324	12.335	-7.349	7.106	1.00	15.47
ATOM	2198	CD2	HIS	A	324	10.200	-7.651	6.762	1.00	16.90
ATOM	2199	CE1	HIS	A	324	11.697	-6.732	8.080	1.00	14.50
ATOM	2200	NE2	HIS	A	324	10.399	-6.900	7.896	1.00	15.07
ATOM	2201	N	ASN	A	325	14.103	-6.864	4.196	1.00	15.06
ATOM	2202	CA	ASN	A	325	15.046	-5.800	4.443	1.00	18.56
ATOM	2203	C	ASN	A	325	15.172	-4.855	3.254	1.00	21.93
ATOM	2204	O	ASN	A	325	15.618	-3.719	3.414	1.00	26.00
ATOM	2205	CB	ASN	A	325	16.420	-6.385	4.789	1.00	19.57
ATOM	2206	CG	ASN	A	325	16.439	-7.076	6.144	1.00	21.82
ATOM	2207	OD1	ASN	A	325	15.416	-7.160	6.831	1.00	21.71
ATOM	2208	ND2	ASN	A	325	17.602	-7.569	6.535	1.00	17.20
ATOM	2209	N	LYS	A	326	14.891	-5.362	2.053	1.00	21.92
ATOM	2210	CA	LYS	A	326	14.954	-4.564	0.838	1.00	17.60
ATOM	2211	C	LYS	A	326	13.714	-3.685	0.769	1.00	15.87
ATOM	2212	O	LYS	A	326	13.785	-2.516	0.392	1.00	15.12
ATOM	2213	CB	LYS	A	326	15.025	-5.462	-0.392	1.00	18.74
ATOM	2214	CG	LYS	A	326	16.361	-6.142	-0.598	1.00	19.18
ATOM	2215	CD	LYS	A	326	16.286	-7.055	-1.796	1.00	18.11
ATOM	2216	CE	LYS	A	326	17.666	-7.461	-2.243	1.00	19.55
ATOM	2217	NZ	LYS	A	326	17.545	-8.481	-3.340	1.00	25.56
ATOM	2218	N	LEU	A	327	12.575	-4.248	1.145	1.00	13.43
ATOM	2219	CA	LEU	A	327	11.338	-3.501	1.145	1.00	14.62
ATOM	2220	C	LEU	A	327	11.329	-2.485	2.302	1.00	17.67
ATOM	2221	O	LEU	A	327	10.752	-1.412	2.196	1.00	19.98
ATOM	2222	CB	LEU	A	327	10.160	-4.461	1.246	1.00	10.36
ATOM	2223	CG	LEU	A	327	8.790	-3.803	1.262	1.00	12.10
ATOM	2224	CD1	LEU	A	327	8.594	-2.894	0.021	1.00	15.96
ATOM	2225	CD2	LEU	A	327	7.731	-4.883	1.328	1.00	12.46
ATOM	2226	N	LYS	A	328	11.992	-2.820	3.396	1.00	17.49
ATOM	2227	CA	LYS	A	328	12.062	-1.932	4.542	1.00	16.76
ATOM	2228	C	LYS	A	328	13.044	-0.790	4.269	1.00	14.85
ATOM	2229	O	LYS	A	328	12.806	0.361	4.647	1.00	15.55
ATOM	2230	CB	LYS	A	328	12.497	-2.723	5.784	1.00	13.97
ATOM	2231	CG	LYS	A	328	11.381	-3.476	6.440	1.00	12.37
ATOM	2232	CD	LYS	A	328	10.266	-2.520	6.773	1.00	15.62
ATOM	2233	CE	LYS	A	328	8.998	-3.236	7.124	1.00	18.22
ATOM	2234	NZ	LYS	A	328	7.928	-2.271	7.511	1.00	27.89
ATOM	2235	N	ALA	A	329	14.135	-1.131	3.596	1.00	11.88
ATOM	2236	CA	ALA	A	329	15.188	-0.194	3.245	1.00	13.33
ATOM	2237	C	ALA	A	329	14.696	0.924	2.333	1.00	14.85
ATOM	2238	O	ALA	A	329	15.270	2.010	2.303	1.00	11.99
ATOM	2239	CB	ALA	A	329	16.340	-0.927	2.592	1.00	12.09

FIG. 2MM

ATOM	2240	N	SER	A	330	13.663	0.621	1.559	1.00	16.65
ATOM	2241	CA	SER	A	330	13.046	1.568	0.647	1.00	20.24
ATOM	2242	C	SER	A	330	12.014	2.374	1.430	1.00	19.37
ATOM	2243	O	SER	A	330	11.680	3.503	1.075	1.00	20.59
ATOM	2244	CB	SER	A	330	12.361	0.820	-0.510	1.00	19.48
ATOM	2245	OG	SER	A	330	11.717	1.714	-1.396	1.00	23.75
ATOM	2246	N	GLN	A	331	11.460	1.762	2.462	1.00	18.23
ATOM	2247	CA	GLN	A	331	10.494	2.442	3.290	1.00	19.23
ATOM	2248	C	GLN	A	331	11.219	3.484	4.124	1.00	19.62
ATOM	2249	O	GLN	A	331	10.726	4.586	4.308	1.00	19.08
ATOM	2250	CB	GLN	A	331	9.787	1.451	4.191	1.00	15.77
ATOM	2251	CG	GLN	A	331	8.474	1.061	3.629	1.00	16.36
ATOM	2252	CD	GLN	A	331	8.030	-0.292	4.087	1.00	14.43
ATOM	2253	OE1	GLN	A	331	8.762	-0.994	4.763	1.00	23.19
ATOM	2254	NE2	GLN	A	331	6.829	-0.673	3.718	1.00	12.76
ATOM	2255	N	ALA	A	332	12.422	3.133	4.562	1.00	19.54
ATOM	2256	CA	ALA	A	332	13.249	3.994	5.384	1.00	19.46
ATOM	2257	C	ALA	A	332	13.761	5.205	4.623	1.00	21.75
ATOM	2258	O	ALA	A	332	13.957	6.266	5.203	1.00	22.56
ATOM	2259	CB	ALA	A	332	14.421	3.207	5.932	1.00	14.44
ATOM	2260	N	ARG	A	333	14.003	5.045	3.331	1.00	21.94
ATOM	2261	CA	ARG	A	333	14.509	6.142	2.536	1.00	22.76
ATOM	2262	C	ARG	A	333	13.390	7.123	2.259	1.00	22.62
ATOM	2263	O	ARG	A	333	13.589	8.332	2.216	1.00	22.94
ATOM	2264	CB	ARG	A	333	15.079	5.628	1.222	1.00	25.59
ATOM	2265	CG	ARG	A	333	16.450	6.149	0.922	1.00	26.01
ATOM	2266	CD	ARG	A	333	16.778	5.976	-0.524	1.00	25.64
ATOM	2267	NE	ARG	A	333	18.026	5.255	-0.680	1.00	32.29
ATOM	2268	CZ	ARG	A	333	18.108	3.936	-0.831	1.00	35.86
ATOM	2269	NH1	ARG	A	333	17.000	3.191	-0.847	1.00	36.93
ATOM	2270	NH2	ARG	A	333	19.299	3.362	-0.992	1.00	39.62
ATOM	2271	N	ASP	A	334	12.191	6.594	2.128	1.00	20.64
ATOM	2272	CA	ASP	A	334	11.054	7.423	1.846	1.00	21.35
ATOM	2273	C	ASP	A	334	10.724	8.307	3.028	1.00	22.23
ATOM	2274	O	ASP	A	334	10.322	9.451	2.846	1.00	24.26
ATOM	2275	CB	ASP	A	334	9.867	6.547	1.526	1.00	22.69
ATOM	2276	CG	ASP	A	334	8.780	7.294	0.836	1.00	21.51
ATOM	2277	OD1	ASP	A	334	8.988	7.667	-0.344	1.00	25.96
ATOM	2278	OD2	ASP	A	334	7.720	7.485	1.469	1.00	23.53
ATOM	2279	N	LEU	A	335	10.852	7.762	4.235	1.00	21.61
ATOM	2280	CA	LEU	A	335	10.564	8.522	5.441	1.00	19.50
ATOM	2281	C	LEU	A	335	11.643	9.582	5.571	1.00	18.55
ATOM	2282	O	LEU	A	335	11.348	10.746	5.840	1.00	17.43
ATOM	2283	CB	LEU	A	335	10.537	7.617	6.681	1.00	17.26
ATOM	2284	CG	LEU	A	335	10.015	8.264	7.977	1.00	16.18
ATOM	2285	CD1	LEU	A	335	8.588	8.746	7.786	1.00	16.01
ATOM	2286	CD2	LEU	A	335	10.076	7.276	9.131	1.00	14.68
ATOM	2287	N	LEU	A	336	12.887	9.179	5.336	1.00	16.64
ATOM	2288	CA	LEU	A	336	14.005	10.086	5.407	1.00	16.93
ATOM	2289	C	LEU	A	336	13.807	11.218	4.413	1.00	19.18
ATOM	2290	O	LEU	A	336	14.043	12.382	4.736	1.00	24.01
ATOM	2291	CB	LEU	A	336	15.299	9.358	5.071	1.00	14.09
ATOM	2292	CG	LEU	A	336	16.249	8.901	6.179	1.00	16.94
ATOM	2293	CD1	LEU	A	336	17.503	8.330	5.565	1.00	10.16
ATOM	2294	CD2	LEU	A	336	16.599	10.075	7.102	1.00	13.20
ATOM	2295	N	SER	A	337	13.315	10.889	3.226	1.00	17.20
ATOM	2296	CA	SER	A	337	13.114	11.882	2.184	1.00	14.95
ATOM	2297	C	SER	A	337	12.032	12.868	2.559	1.00	13.10
ATOM	2298	O	SER	A	337	12.090	14.025	2.158	1.00	15.70

FIG. 2NN

ATOM	2299	CB	SER	A	337	12.837	11.222	0.800	1.00	9.08
ATOM	2300	OG	SER	A	337	11.455	11.067	0.520	1.00	6.87
ATOM	2301	N	LYS	A	338	11.060	12.421	3.344	1.00	12.04
ATOM	2302	CA	LYS	A	338	9.962	13.281	3.764	1.00	12.08
ATOM	2303	C	LYS	A	338	10.242	14.118	5.032	1.00	14.69
ATOM	2304	O	LYS	A	338	9.586	15.131	5.295	1.00	11.13
ATOM	2305	CB	LYS	A	338	8.733	12.429	3.990	1.00	12.09
ATOM	2306	CG	LYS	A	338	8.203	11.758	2.763	1.00	12.08
ATOM	2307	CD	LYS	A	338	7.002	10.919	3.111	1.00	12.89
ATOM	2308	CE	LYS	A	338	6.220	10.601	1.882	1.00	20.87
ATOM	2309	NZ	LYS	A	338	7.157	10.324	0.750	1.00	24.91
ATOM	2310	N	MET	A	339	11.216	13.666	5.814	1.00	16.21
ATOM	2311	CA	MET	A	339	11.600	14.310	7.046	1.00	16.11
ATOM	2312	C	MET	A	339	12.691	15.354	6.832	1.00	16.02
ATOM	2313	O	MET	A	339	12.602	16.458	7.374	1.00	17.20
ATOM	2314	CB	MET	A	339	12.075	13.260	8.066	1.00	17.91
ATOM	2315	CG	MET	A	339	11.016	12.221	8.487	1.00	15.40
ATOM	2316	SD	MET	A	339	11.399	11.344	10.070	1.00	11.13
ATOM	2317	CE	MET	A	339	9.803	10.977	10.535	1.00	4.76
ATOM	2318	N	LEU	A	340	13.745	14.995	6.102	1.00	13.03
ATOM	2319	CA	LEU	A	340	14.815	15.942	5.847	1.00	9.12
ATOM	2320	C	LEU	A	340	14.414	16.893	4.749	1.00	9.02
ATOM	2321	O	LEU	A	340	14.950	16.822	3.655	1.00	11.54
ATOM	2322	CB	LEU	A	340	16.112	15.232	5.464	1.00	10.00
ATOM	2323	CG	LEU	A	340	16.730	14.338	6.536	1.00	13.72
ATOM	2324	CD1	LEU	A	340	18.045	13.775	6.031	1.00	13.72
ATOM	2325	CD2	LEU	A	340	16.945	15.144	7.815	1.00	12.06
ATOM	2326	N	VAL	A	341	13.399	17.708	5.002	1.00	10.15
ATOM	2327	CA	VAL	A	341	12.947	18.693	4.029	1.00	16.38
ATOM	2328	C	VAL	A	341	13.129	20.074	4.642	1.00	18.38
ATOM	2329	O	VAL	A	341	12.477	20.393	5.620	1.00	20.26
ATOM	2330	CB	VAL	A	341	11.472	18.547	3.681	1.00	15.80
ATOM	2331	CG1	VAL	A	341	11.198	19.269	2.396	1.00	12.46
ATOM	2332	CG2	VAL	A	341	11.086	17.106	3.565	1.00	21.60
ATOM	2333	N	ILE	A	342	13.968	20.909	4.040	1.00	21.30
ATOM	2334	CA	ILE	A	342	14.224	22.252	4.559	1.00	23.13
ATOM	2335	C	ILE	A	342	12.966	23.094	4.698	1.00	22.57
ATOM	2336	O	ILE	A	342	12.845	23.856	5.650	1.00	24.81
ATOM	2337	CB	ILE	A	342	15.260	23.013	3.704	1.00	24.58
ATOM	2338	CG1	ILE	A	342	16.591	22.252	3.691	1.00	21.38
ATOM	2339	CG2	ILE	A	342	15.415	24.473	4.213	1.00	28.32
ATOM	2340	CD1	ILE	A	342	17.637	22.857	2.776	1.00	21.55
ATOM	2341	N	ASP	A	343	12.004	22.931	3.801	1.00	20.64
ATOM	2342	CA	ASP	A	343	10.797	23.719	3.911	1.00	18.43
ATOM	2343	C	ASP	A	343	9.741	23.050	4.789	1.00	19.72
ATOM	2344	O	ASP	A	343	9.096	22.110	4.364	1.00	22.83
ATOM	2345	CB	ASP	A	343	10.249	23.984	2.514	1.00	19.98
ATOM	2346	CG	ASP	A	343	9.077	24.953	2.510	1.00	22.57
ATOM	2347	OD1	ASP	A	343	8.332	25.008	3.492	1.00	23.19
ATOM	2348	OD2	ASP	A	343	8.872	25.667	1.508	1.00	26.66
ATOM	2349	N	PRO	A	344	9.475	23.596	5.990	1.00	20.20
ATOM	2350	CA	PRO	A	344	8.470	23.018	6.894	1.00	16.72
ATOM	2351	C	PRO	A	344	7.086	22.922	6.304	1.00	18.97
ATOM	2352	O	PRO	A	344	6.211	22.252	6.854	1.00	19.62
ATOM	2353	CB	PRO	A	344	8.479	23.987	8.075	1.00	17.59
ATOM	2354	CG	PRO	A	344	8.911	25.278	7.461	1.00	17.94
ATOM	2355	CD	PRO	A	344	10.034	24.826	6.574	1.00	18.08
ATOM	2356	N	ALA	A	345	6.862	23.674	5.235	1.00	19.74
ATOM	2357	CA	ALA	A	345	5.583	23.694	4.548	1.00	18.23

FIG. 200

ATOM	2358	C	ALA	A	345	5.453	22.445	3.724	1.00	17.55
ATOM	2359	O	ALA	A	345	4.350	22.043	3.381	1.00	19.09
ATOM	2360	CB	ALA	A	345	5.458	24.927	3.659	1.00	18.19
ATOM	2361	N	LYS	A	346	6.589	21.831	3.420	1.00	18.76
ATOM	2362	CA	LYS	A	346	6.635	20.590	2.653	1.00	22.13
ATOM	2363	C	LYS	A	346	7.160	19.356	3.444	1.00	22.18
ATOM	2364	O	LYS	A	346	7.104	18.231	2.952	1.00	22.05
ATOM	2365	CB	LYS	A	346	7.468	20.811	1.385	1.00	26.61
ATOM	2366	CG	LYS	A	346	6.903	21.904	0.471	1.00	33.55
ATOM	2367	CD	LYS	A	346	7.743	22.051	-0.789	1.00	38.48
ATOM	2368	CE	LYS	A	346	7.883	20.707	-1.515	1.00	43.70
ATOM	2369	NZ	LYS	A	346	8.631	20.765	-2.819	1.00	47.82
ATOM	2370	N	ARG	A	347	7.648	19.575	4.664	1.00	19.68
ATOM	2371	CA	ARG	A	347	8.174	18.519	5.527	1.00	17.00
ATOM	2372	C	ARG	A	347	7.004	17.683	6.064	1.00	16.03
ATOM	2373	O	ARG	A	347	5.874	18.151	6.082	1.00	15.59
ATOM	2374	CB	ARG	A	347	8.956	19.158	6.678	1.00	16.04
ATOM	2375	CG	ARG	A	347	9.829	18.222	7.483	1.00	15.84
ATOM	2376	CD	ARG	A	347	10.449	18.926	8.675	1.00	16.35
ATOM	2377	NE	ARG	A	347	11.419	19.939	8.266	1.00	17.58
ATOM	2378	CZ	ARG	A	347	11.472	21.176	8.757	1.00	16.09
ATOM	2379	NH1	ARG	A	347	10.606	21.553	9.680	1.00	18.02
ATOM	2380	NH2	ARG	A	347	12.385	22.042	8.319	1.00	14.89
ATOM	2381	N	ILE	A	348	7.254	16.437	6.466	1.00	16.76
ATOM	2382	CA	ILE	A	348	6.180	15.575	6.984	1.00	16.86
ATOM	2383	C	ILE	A	348	5.909	15.867	8.466	1.00	17.05
ATOM	2384	O	ILE	A	348	6.805	16.319	9.180	1.00	18.30
ATOM	2385	CB	ILE	A	348	6.484	14.031	6.734	1.00	18.03
ATOM	2386	CG1	ILE	A	348	5.235	13.195	6.988	1.00	19.19
ATOM	2387	CG2	ILE	A	348	7.610	13.523	7.608	1.00	12.85
ATOM	2388	CD1	ILE	A	348	5.455	11.731	6.750	1.00	22.05
ATOM	2389	N	SER	A	349	4.666	15.651	8.901	1.00	15.54
ATOM	2390	CA	SER	A	349	4.257	15.912	10.273	1.00	15.42
ATOM	2391	C	SER	A	349	4.443	14.695	11.187	1.00	18.21
ATOM	2392	O	SER	A	349	4.959	13.665	10.748	1.00	19.66
ATOM	2393	CB	SER	A	349	2.808	16.395	10.297	1.00	13.74
ATOM	2394	OG	SER	A	349	1.896	15.362	9.984	1.00	15.03
ATOM	2395	N	VAL	A	350	4.047	14.821	12.460	1.00	20.51
ATOM	2396	CA	VAL	A	350	4.198	13.738	13.447	1.00	18.94
ATOM	2397	C	VAL	A	350	3.147	12.664	13.230	1.00	16.49
ATOM	2398	O	VAL	A	350	3.446	11.478	13.336	1.00	18.02
ATOM	2399	CB	VAL	A	350	4.083	14.250	14.941	1.00	19.83
ATOM	2400	CG1	VAL	A	350	4.553	13.183	15.922	1.00	14.18
ATOM	2401	CG2	VAL	A	350	4.893	15.506	15.153	1.00	19.35
ATOM	2402	N	ASP	A	351	1.928	13.087	12.912	1.00	15.82
ATOM	2403	CA	ASP	A	351	0.821	12.167	12.696	1.00	19.48
ATOM	2404	C	ASP	A	351	0.886	11.383	11.404	1.00	21.44
ATOM	2405	O	ASP	A	351	0.288	10.322	11.289	1.00	24.24
ATOM	2406	CB	ASP	A	351	-0.517	12.896	12.802	1.00	19.34
ATOM	2407	CG	ASP	A	351	-0.818	13.346	14.216	1.00	22.25
ATOM	2408	OD1	ASP	A	351	-1.880	13.959	14.447	1.00	21.31
ATOM	2409	OD2	ASP	A	351	0.014	13.083	15.108	1.00	23.43
ATOM	2410	N	ASP	A	352	1.568	11.922	10.409	1.00	21.74
ATOM	2411	CA	ASP	A	352	1.699	11.221	9.152	1.00	20.56
ATOM	2412	C	ASP	A	352	2.953	10.380	9.214	1.00	19.06
ATOM	2413	O	ASP	A	352	3.059	9.378	8.516	1.00	20.14
ATOM	2414	CB	ASP	A	352	1.797	12.191	7.967	1.00	21.74
ATOM	2415	CG	ASP	A	352	0.504	12.922	7.680	1.00	20.06
ATOM	2416	OD1	ASP	A	352	-0.591	12.512	8.148	1.00	19.05

FIG. 2PP

ATOM	2417	OD2	ASP	A	352	0.597	13.925	6.961	1.00	21.55
ATOM	2418	N	ALA	A	353	3.925	10.819	10.002	1.00	16.38
ATOM	2419	CA	ALA	A	353	5.154	10.082	10.141	1.00	15.27
ATOM	2420	C	ALA	A	353	4.845	8.814	10.954	1.00	18.82
ATOM	2421	O	ALA	A	353	5.497	7.791	10.778	1.00	20.49
ATOM	2422	CB	ALA	A	353	6.240	10.943	10.789	1.00	9.63
ATOM	2423	N	LEU	A	354	3.791	8.854	11.766	1.00	19.59
ATOM	2424	CA	LEU	A	354	3.397	7.699	12.567	1.00	20.91
ATOM	2425	C	LEU	A	354	2.625	6.687	11.738	1.00	22.39
ATOM	2426	O	LEU	A	354	2.633	5.487	12.044	1.00	22.66
ATOM	2427	CB	LEU	A	354	2.581	8.144	13.782	1.00	20.28
ATOM	2428	CG	LEU	A	354	3.366	8.623	15.027	1.00	22.16
ATOM	2429	CD1	LEU	A	354	2.518	9.564	15.886	1.00	18.21
ATOM	2430	CD2	LEU	A	354	3.837	7.427	15.847	1.00	18.64
ATOM	2431	N	GLN	A	355	1.974	7.189	10.682	1.00	25.01
ATOM	2432	CA	GLN	A	355	1.193	6.385	9.732	1.00	24.82
ATOM	2433	C	GLN	A	355	1.964	6.083	8.427	1.00	24.07
ATOM	2434	O	GLN	A	355	1.387	5.761	7.391	1.00	23.85
ATOM	2435	CB	GLN	A	355	-0.165	7.040	9.446	1.00	26.02
ATOM	2436	CG	GLN	A	355	-1.104	7.110	10.653	1.00	31.50
ATOM	2437	CD	GLN	A	355	-1.522	5.738	11.190	1.00	37.67
ATOM	2438	OE1	GLN	A	355	-0.731	4.777	11.217	1.00	41.39
ATOM	2439	NE2	GLN	A	355	-2.758	5.654	11.670	1.00	41.86
ATOM	2440	N	HIS	A	356	3.283	6.231	8.494	1.00	24.42
ATOM	2441	CA	HIS	A	356	4.169	5.916	7.385	1.00	22.45
ATOM	2442	C	HIS	A	356	4.396	4.424	7.609	1.00	24.49
ATOM	2443	O	HIS	A	356	4.648	3.996	8.729	1.00	24.40
ATOM	2444	CB	HIS	A	356	5.504	6.643	7.550	1.00	18.90
ATOM	2445	CG	HIS	A	356	6.447	6.466	6.397	1.00	19.41
ATOM	2446	ND1	HIS	A	356	6.368	7.226	5.249	1.00	17.71
ATOM	2447	CD2	HIS	A	356	7.524	5.665	6.243	1.00	16.97
ATOM	2448	CE1	HIS	A	356	7.359	6.902	4.439	1.00	13.61
ATOM	2449	NE2	HIS	A	356	8.075	5.960	5.020	1.00	17.38
ATOM	2450	N	PRO	A	357	4.337	3.619	6.544	1.00	25.58
ATOM	2451	CA	PRO	A	357	4.538	2.170	6.656	1.00	22.18
ATOM	2452	C	PRO	A	357	5.804	1.715	7.393	1.00	19.11
ATOM	2453	O	PRO	A	357	5.829	0.608	7.939	1.00	23.70
ATOM	2454	CB	PRO	A	357	4.542	1.711	5.187	1.00	23.59
ATOM	2455	CG	PRO	A	357	4.997	2.946	4.429	1.00	23.68
ATOM	2456	CD	PRO	A	357	4.204	4.025	5.136	1.00	24.01
ATOM	2457	N	TYR	A	358	6.855	2.523	7.407	1.00	13.73
ATOM	2458	CA	TYR	A	358	8.066	2.108	8.086	1.00	10.20
ATOM	2459	C	TYR	A	358	7.921	2.208	9.627	1.00	15.75
ATOM	2460	O	TYR	A	358	8.742	1.650	10.365	1.00	14.80
ATOM	2461	CB	TYR	A	358	9.233	2.964	7.622	1.00	6.07
ATOM	2462	CG	TYR	A	358	10.577	2.532	8.168	1.00	6.30
ATOM	2463	CD1	TYR	A	358	11.287	1.528	7.563	1.00	8.94
ATOM	2464	CD2	TYR	A	358	11.151	3.145	9.282	1.00	8.80
ATOM	2465	CE1	TYR	A	358	12.534	1.137	8.043	1.00	9.47
ATOM	2466	CE2	TYR	A	358	12.409	2.746	9.773	1.00	8.25
ATOM	2467	CZ	TYR	A	358	13.094	1.735	9.144	1.00	5.06
ATOM	2468	OH	TYR	A	358	14.339	1.288	9.583	1.00	4.74
ATOM	2469	N	ILE	A	359	6.863	2.889	10.090	1.00	15.98
ATOM	2470	CA	ILE	A	359	6.613	3.122	11.511	1.00	16.40
ATOM	2471	C	ILE	A	359	5.243	2.683	12.004	1.00	18.15
ATOM	2472	O	ILE	A	359	5.088	2.415	13.193	1.00	24.14
ATOM	2473	CB	ILE	A	359	6.714	4.649	11.863	1.00	15.03
ATOM	2474	CG1	ILE	A	359	8.015	5.245	11.354	1.00	11.94
ATOM	2475	CG2	ILE	A	359	6.567	4.874	13.352	1.00	11.43

FIG. 2QQ

ATOM	2476	CD1	ILE	A	359	9.183	4.972	12.216	1.00	12.83
ATOM	2477	N	ASN	A	360	4.240	2.632	11.136	1.00	19.28
ATOM	2478	CA	ASN	A	360	2.912	2.249	11.601	1.00	21.24
ATOM	2479	C	ASN	A	360	2.808	0.778	12.026	1.00	19.53
ATOM	2480	O	ASN	A	360	1.857	0.391	12.691	1.00	21.14
ATOM	2481	CB	ASN	A	360	1.798	2.659	10.602	1.00	24.74
ATOM	2482	CG	ASN	A	360	1.637	1.685	9.438	1.00	28.99
ATOM	2483	OD1	ASN	A	360	2.619	1.150	8.913	1.00	34.08
ATOM	2484	ND2	ASN	A	360	0.396	1.473	9.016	1.00	28.15
ATOM	2485	N	VAL	A	361	3.805	-0.033	11.702	1.00	18.76
ATOM	2486	CA	VAL	A	361	3.753	-1.434	12.112	1.00	23.04
ATOM	2487	C	VAL	A	361	3.727	-1.557	13.641	1.00	26.35
ATOM	2488	O	VAL	A	361	3.186	-2.523	14.171	1.00	29.64
ATOM	2489	CB	VAL	A	361	4.954	-2.258	11.594	1.00	19.01
ATOM	2490	CG1	VAL	A	361	5.002	-2.250	10.067	1.00	20.77
ATOM	2491	CG2	VAL	A	361	6.240	-1.751	12.205	1.00	18.11
ATOM	2492	N	TRP	A	362	4.279	-0.561	14.342	1.00	28.15
ATOM	2493	CA	TRP	A	362	4.333	-0.541	15.811	1.00	24.02
ATOM	2494	C	TRP	A	362	3.253	0.314	16.440	1.00	22.25
ATOM	2495	O	TRP	A	362	3.133	0.352	17.650	1.00	28.38
ATOM	2496	CB	TRP	A	362	5.643	0.060	16.272	1.00	19.04
ATOM	2497	CG	TRP	A	362	6.805	-0.610	15.778	1.00	19.63
ATOM	2498	CD1	TRP	A	362	7.701	-0.128	14.872	1.00	21.93
ATOM	2499	CD2	TRP	A	362	7.343	-1.829	16.281	1.00	21.65
ATOM	2500	NE1	TRP	A	362	8.790	-0.961	14.801	1.00	21.62
ATOM	2501	CE2	TRP	A	362	8.597	-2.014	15.659	1.00	22.35
ATOM	2502	CE3	TRP	A	362	6.900	-2.769	17.206	1.00	20.16
ATOM	2503	CZ2	TRP	A	362	9.416	-3.113	15.957	1.00	20.95
ATOM	2504	CZ3	TRP	A	362	7.706	-3.841	17.498	1.00	16.39
ATOM	2505	CH2	TRP	A	362	8.949	-4.010	16.880	1.00	15.82
ATOM	2506	N	TYR	A	363	2.479	1.003	15.627	1.00	22.86
ATOM	2507	CA	TYR	A	363	1.453	1.910	16.095	1.00	24.69
ATOM	2508	C	TYR	A	363	0.492	1.297	17.097	1.00	28.12
ATOM	2509	O	TYR	A	363	0.109	0.134	16.954	1.00	30.75
ATOM	2510	CB	TYR	A	363	0.704	2.489	14.892	1.00	26.24
ATOM	2511	CG	TYR	A	363	-0.318	3.529	15.234	1.00	26.14
ATOM	2512	CD1	TYR	A	363	-1.647	3.188	15.408	1.00	26.69
ATOM	2513	CD2	TYR	A	363	0.043	4.856	15.405	1.00	28.71
ATOM	2514	CE1	TYR	A	363	-2.579	4.129	15.740	1.00	27.93
ATOM	2515	CE2	TYR	A	363	-0.898	5.809	15.744	1.00	26.78
ATOM	2516	CZ	TYR	A	363	-2.198	5.432	15.905	1.00	25.74
ATOM	2517	OH	TYR	A	363	-3.151	6.353	16.213	1.00	33.01
ATOM	2518	N	ASP	A	364	0.072	2.115	18.074	1.00	28.98
ATOM	2519	CA	ASP	A	364	-0.834	1.718	19.152	1.00	26.46
ATOM	2520	C	ASP	A	364	-1.577	2.952	19.654	1.00	26.25
ATOM	2521	O	ASP	A	364	-0.975	3.880	20.160	1.00	29.14
ATOM	2522	CB	ASP	A	364	-0.019	1.089	20.295	1.00	24.81
ATOM	2523	CG	ASP	A	364	-0.881	0.569	21.439	1.00	27.58
ATOM	2524	OD1	ASP	A	364	-2.074	0.932	21.541	1.00	28.14
ATOM	2525	OD2	ASP	A	364	-0.355	-0.201	22.268	1.00	34.84
ATOM	2526	N	PRO	A	365	-2.897	2.968	19.534	1.00	25.78
ATOM	2527	CA	PRO	A	365	-3.661	4.119	20.000	1.00	28.64
ATOM	2528	C	PRO	A	365	-3.331	4.580	21.408	1.00	30.94
ATOM	2529	O	PRO	A	365	-2.838	5.690	21.581	1.00	33.56
ATOM	2530	CB	PRO	A	365	-5.098	3.641	19.849	1.00	27.83
ATOM	2531	CG	PRO	A	365	-5.014	2.875	18.555	1.00	27.49
ATOM	2532	CD	PRO	A	365	-3.752	2.049	18.773	1.00	28.07
ATOM	2533	N	ALA	A	366	-3.539	3.725	22.406	1.00	33.50
ATOM	2534	CA	ALA	A	366	-3.254	4.086	23.802	1.00	34.17

FIG. 2RR

ATOM	2535	C	ALA	A	366	-1.828	4.610	23.995	1.00	34.01
ATOM	2536	O	ALA	A	366	-1.583	5.519	24.792	1.00	33.18
ATOM	2537	CB	ALA	A	366	-3.490	2.885	24.701	1.00	38.15
ATOM	2538	N	GLU	A	367	-0.913	4.046	23.215	1.00	34.87
ATOM	2539	CA	GLU	A	367	0.508	4.384	23.223	1.00	35.12
ATOM	2540	C	GLU	A	367	0.799	5.663	22.429	1.00	36.01
ATOM	2541	O	GLU	A	367	1.846	6.286	22.597	1.00	34.03
ATOM	2542	CB	GLU	A	367	1.283	3.229	22.607	1.00	36.74
ATOM	2543	CG	GLU	A	367	2.622	2.921	23.231	1.00	37.45
ATOM	2544	CD	GLU	A	367	3.323	1.742	22.543	1.00	37.93
ATOM	2545	OE1	GLU	A	367	3.056	1.476	21.340	1.00	34.38
ATOM	2546	OE2	GLU	A	367	4.148	1.082	23.206	1.00	38.70
ATOM	2547	N	VAL	A	368	-0.136	6.058	21.572	1.00	37.78
ATOM	2548	CA	VAL	A	368	0.034	7.262	20.774	1.00	38.83
ATOM	2549	C	VAL	A	368	-0.925	8.387	21.186	1.00	39.06
ATOM	2550	O	VAL	A	368	-0.473	9.434	21.642	1.00	41.85
ATOM	2551	CB	VAL	A	368	-0.076	6.978	19.243	1.00	37.06
ATOM	2552	CG1	VAL	A	368	-0.058	8.277	18.463	1.00	37.21
ATOM	2553	CG2	VAL	A	368	1.072	6.123	18.786	1.00	35.19
ATOM	2554	N	GLU	A	369	-2.233	8.197	21.011	1.00	40.22
ATOM	2555	CA	GLU	A	369	-3.195	9.241	21.377	1.00	42.42
ATOM	2556	C	GLU	A	369	-3.801	9.073	22.753	1.00	42.83
ATOM	2557	O	GLU	A	369	-4.960	8.673	22.915	1.00	42.26
ATOM	2558	CB	GLU	A	369	-4.294	9.438	20.319	1.00	44.75
ATOM	2559	CG	GLU	A	369	-5.014	8.180	19.855	1.00	45.12
ATOM	2560	CD	GLU	A	369	-4.439	7.620	18.561	1.00	46.29
ATOM	2561	OE1	GLU	A	369	-3.313	8.031	18.196	1.00	44.38
ATOM	2562	OE2	GLU	A	369	-5.115	6.774	17.922	1.00	44.39
ATOM	2563	N	ALA	A	370	-3.013	9.494	23.731	1.00	44.29
ATOM	2564	CA	ALA	A	370	-3.378	9.420	25.126	1.00	45.80
ATOM	2565	C	ALA	A	370	-3.316	10.812	25.750	1.00	46.17
ATOM	2566	O	ALA	A	370	-2.472	11.639	25.373	1.00	44.23
ATOM	2567	CB	ALA	A	370	-2.430	8.464	25.860	1.00	47.56
ATOM	2568	N	PRO	A	371	-4.234	11.086	26.695	1.00	47.08
ATOM	2569	CA	PRO	A	371	-4.333	12.370	27.412	1.00	47.97
ATOM	2570	C	PRO	A	371	-3.001	12.746	28.091	1.00	47.33
ATOM	2571	O	PRO	A	371	-2.308	11.887	28.651	1.00	48.84
ATOM	2572	CB	PRO	A	371	-5.446	12.091	28.438	1.00	47.47
ATOM	2573	CG	PRO	A	371	-6.343	11.117	27.704	1.00	46.69
ATOM	2574	CD	PRO	A	371	-5.312	10.173	27.119	1.00	46.13
ATOM	2575	N	PRO	A	372	-2.584	14.030	27.959	1.00	44.53
ATOM	2576	CA	PRO	A	372	-1.351	14.560	28.557	1.00	43.72
ATOM	2577	C	PRO	A	372	-1.247	14.823	30.092	1.00	43.15
ATOM	2578	O	PRO	A	372	-0.392	14.225	30.755	1.00	38.33
ATOM	2579	CB	PRO	A	372	-1.060	15.805	27.692	1.00	42.06
ATOM	2580	CG	PRO	A	372	-2.418	16.198	27.182	1.00	43.54
ATOM	2581	CD	PRO	A	372	-3.031	14.874	26.844	1.00	41.44
ATOM	2582	N	PRO	A	373	-2.124	15.680	30.688	1.00	45.40
ATOM	2583	CA	PRO	A	373	-1.991	15.905	32.142	1.00	48.11
ATOM	2584	C	PRO	A	373	-2.838	14.972	33.035	1.00	48.84
ATOM	2585	O	PRO	A	373	-3.957	15.358	33.472	1.00	47.99
ATOM	2586	CB	PRO	A	373	-2.406	17.394	32.305	1.00	48.09
ATOM	2587	CG	PRO	A	373	-2.950	17.835	30.926	1.00	45.71
ATOM	2588	CD	PRO	A	373	-3.203	16.528	30.171	1.00	46.49
ATOM	2589	N	ALA	A	379	5.622	28.512	36.170	1.00	42.15
ATOM	2590	CA	ALA	A	379	4.671	27.944	35.176	1.00	45.12
ATOM	2591	C	ALA	A	379	5.052	28.375	33.747	1.00	47.76
ATOM	2592	O	ALA	A	379	5.397	27.528	32.908	1.00	47.42
ATOM	2593	CB	ALA	A	379	3.230	28.364	35.511	1.00	42.23

FIG. 2SS

ATOM	2594	N	LEU	A	380	5.012	29.690	33.494	1.00	48.53
ATOM	2595	CA	LEU	A	380	5.343	30.273	32.190	1.00	46.22
ATOM	2596	C	LEU	A	380	6.861	30.312	32.046	1.00	48.02
ATOM	2597	O	LEU	A	380	7.522	31.138	32.662	1.00	47.82
ATOM	2598	CB	LEU	A	380	4.761	31.685	32.081	1.00	43.91
ATOM	2599	CG	LEU	A	380	3.255	31.846	31.837	1.00	41.45
ATOM	2600	CD1	LEU	A	380	2.852	31.153	30.529	1.00	43.02
ATOM	2601	CD2	LEU	A	380	2.464	31.288	32.988	1.00	37.93
ATOM	2602	N	ASP	A	381	7.398	29.437	31.194	1.00	51.88
ATOM	2603	CA	ASP	A	381	8.853	29.317	31.012	1.00	53.94
ATOM	2604	C	ASP	A	381	9.538	29.929	29.770	1.00	54.51
ATOM	2605	O	ASP	A	381	10.041	29.214	28.892	1.00	53.90
ATOM	2606	CB	ASP	A	381	9.263	27.839	31.152	1.00	57.15
ATOM	2607	CG	ASP	A	381	8.520	27.109	32.277	1.00	58.25
ATOM	2608	OD1	ASP	A	381	8.731	27.455	33.464	1.00	61.41
ATOM	2609	OD2	ASP	A	381	7.735	26.177	31.974	1.00	54.54
ATOM	2610	N	ALA	A	382	9.616	31.254	29.747	1.00	54.88
ATOM	2611	CA	ALA	A	382	10.269	32.050	28.702	1.00	53.46
ATOM	2612	C	ALA	A	382	10.336	33.434	29.382	1.00	54.54
ATOM	2613	O	ALA	A	382	10.287	34.510	28.755	1.00	53.71
ATOM	2614	CB	ALA	A	382	9.405	32.084	27.459	1.00	55.53
ATOM	2615	N	ARG	A	383	10.481	33.331	30.700	1.00	52.53
ATOM	2616	CA	ARG	A	383	10.518	34.404	31.679	1.00	48.12
ATOM	2617	C	ARG	A	383	11.868	35.088	31.895	1.00	45.65
ATOM	2618	O	ARG	A	383	12.817	34.867	31.135	1.00	43.32
ATOM	2619	CB	ARG	A	383	10.037	33.784	32.991	1.00	48.15
ATOM	2620	CG	ARG	A	383	10.757	32.453	33.300	1.00	47.01
ATOM	2621	CD	ARG	A	383	9.897	31.495	34.099	1.00	45.98
ATOM	2622	NE	ARG	A	383	9.381	32.145	35.294	1.00	46.34
ATOM	2623	CZ	ARG	A	383	8.271	31.795	35.935	1.00	45.23
ATOM	2624	NH1	ARG	A	383	7.531	30.776	35.516	1.00	46.97
ATOM	2625	NH2	ARG	A	383	7.863	32.517	36.969	1.00	45.75
ATOM	2626	N	GLU	A	384	11.908	35.937	32.932	1.00	43.92
ATOM	2627	CA	GLU	A	384	13.102	36.688	33.357	1.00	41.03
ATOM	2628	C	GLU	A	384	13.135	36.865	34.895	1.00	38.41
ATOM	2629	O	GLU	A	384	12.148	37.306	35.505	1.00	34.88
ATOM	2630	CB	GLU	A	384	13.102	38.080	32.742	1.00	45.48
ATOM	2631	CG	GLU	A	384	12.783	38.134	31.257	1.00	49.70
ATOM	2632	CD	GLU	A	384	12.403	39.535	30.785	1.00	50.64
ATOM	2633	OE1	GLU	A	384	11.756	40.279	31.567	1.00	47.57
ATOM	2634	OE2	GLU	A	384	12.746	39.874	29.625	1.00	53.02
ATOM	2635	N	HIS	A	385	14.273	36.521	35.504	1.00	34.45
ATOM	2636	CA	HIS	A	385	14.468	36.644	36.950	1.00	30.28
ATOM	2637	C	HIS	A	385	15.931	36.683	37.261	1.00	28.54
ATOM	2638	O	HIS	A	385	16.776	36.326	36.445	1.00	24.90
ATOM	2639	CB	HIS	A	385	13.917	35.454	37.737	1.00	27.07
ATOM	2640	CG	HIS	A	385	12.457	35.211	37.565	1.00	26.81
ATOM	2641	ND1	HIS	A	385	11.504	35.855	38.314	1.00	27.05
ATOM	2642	CD2	HIS	A	385	11.790	34.342	36.766	1.00	28.23
ATOM	2643	CE1	HIS	A	385	10.304	35.396	37.990	1.00	31.75
ATOM	2644	NE2	HIS	A	385	10.452	34.475	37.053	1.00	30.36
ATOM	2645	N	THR	A	386	16.226	37.132	38.468	1.00	32.82
ATOM	2646	CA	THR	A	386	17.602	37.177	38.935	1.00	35.29
ATOM	2647	C	THR	A	386	17.958	35.861	39.623	1.00	33.04
ATOM	2648	O	THR	A	386	17.071	35.101	40.016	1.00	30.47
ATOM	2649	CB	THR	A	386	17.880	38.345	39.907	1.00	37.45
ATOM	2650	OG1	THR	A	386	19.164	38.132	40.515	1.00	43.91
ATOM	2651	CG2	THR	A	386	16.801	38.441	40.989	1.00	36.33
ATOM	2652	N	ILE	A	387	19.257	35.644	39.823	1.00	31.86

FIG. 2TT

ATOM	2653	CA	ILE	A	387	19.776	34.421	40.423	1.00	33.58
ATOM	2654	C	ILE	A	387	19.300	34.068	41.830	1.00	33.37
ATOM	2655	O	ILE	A	387	19.481	32.932	42.285	1.00	31.92
ATOM	2656	CB	ILE	A	387	21.315	34.393	40.388	1.00	35.68
ATOM	2657	CG1	ILE	A	387	21.903	35.487	41.286	1.00	33.18
ATOM	2658	CG2	ILE	A	387	21.789	34.535	38.940	1.00	35.90
ATOM	2659	CD1	ILE	A	387	23.412	35.408	41.424	1.00	29.75
ATOM	2660	N	GLU	A	388	18.756	35.049	42.545	1.00	33.15
ATOM	2661	CA	GLU	A	388	18.247	34.784	43.873	1.00	30.07
ATOM	2662	C	GLU	A	388	16.758	34.593	43.744	1.00	28.18
ATOM	2663	O	GLU	A	388	16.124	33.879	44.518	1.00	26.25
ATOM	2664	CB	GLU	A	388	18.650	35.897	44.828	1.00	35.56
ATOM	2665	CG	GLU	A	388	20.174	35.911	45.063	1.00	42.10
ATOM	2666	CD	GLU	A	388	20.759	34.510	45.329	1.00	45.57
ATOM	2667	OE1	GLU	A	388	20.380	33.900	46.358	1.00	49.57
ATOM	2668	OE2	GLU	A	388	21.599	34.017	44.521	1.00	49.11
ATOM	2669	N	GLU	A	389	16.202	35.192	42.708	1.00	25.49
ATOM	2670	CA	GLU	A	389	14.795	34.998	42.442	1.00	25.44
ATOM	2671	C	GLU	A	389	14.595	33.610	41.785	1.00	23.41
ATOM	2672	O	GLU	A	389	13.521	33.006	41.896	1.00	22.43
ATOM	2673	CB	GLU	A	389	14.270	36.103	41.549	1.00	27.39
ATOM	2674	CG	GLU	A	389	13.547	37.123	42.355	1.00	31.98
ATOM	2675	CD	GLU	A	389	12.863	38.134	41.501	1.00	37.60
ATOM	2676	OE1	GLU	A	389	11.630	37.982	41.322	1.00	40.54
ATOM	2677	OE2	GLU	A	389	13.547	39.082	41.024	1.00	36.37
ATOM	2678	N	TRP	A	390	15.640	33.113	41.124	1.00	18.95
ATOM	2679	CA	TRP	A	390	15.605	31.808	40.491	1.00	17.65
ATOM	2680	C	TRP	A	390	15.715	30.735	41.576	1.00	17.48
ATOM	2681	O	TRP	A	390	14.966	29.767	41.597	1.00	19.35
ATOM	2682	CB	TRP	A	390	16.772	31.673	39.516	1.00	15.00
ATOM	2683	CG	TRP	A	390	16.485	32.149	38.147	1.00	12.48
ATOM	2684	CD1	TRP	A	390	17.300	32.923	37.376	1.00	13.71
ATOM	2685	CD2	TRP	A	390	15.310	31.882	37.357	1.00	11.84
ATOM	2686	NE1	TRP	A	390	16.706	33.166	36.157	1.00	13.62
ATOM	2687	CE2	TRP	A	390	15.485	32.538	36.118	1.00	11.97
ATOM	2688	CE3	TRP	A	390	14.142	31.151	37.569	1.00	14.72
ATOM	2689	CZ2	TRP	A	390	14.529	32.486	35.104	1.00	11.62
ATOM	2690	CZ3	TRP	A	390	13.186	31.099	36.553	1.00	14.87
ATOM	2691	CH2	TRP	A	390	13.386	31.759	35.338	1.00	11.15
ATOM	2692	N	LYS	A	391	16.651	30.941	42.490	1.00	20.23
ATOM	2693	CA	LYS	A	391	16.888	30.049	43.607	1.00	20.65
ATOM	2694	C	LYS	A	391	15.601	29.802	44.400	1.00	22.95
ATOM	2695	O	LYS	A	391	15.301	28.654	44.748	1.00	24.92
ATOM	2696	CB	LYS	A	391	17.988	30.651	44.471	1.00	21.29
ATOM	2697	CG	LYS	A	391	18.444	29.831	45.640	1.00	20.35
ATOM	2698	CD	LYS	A	391	19.809	30.312	46.095	1.00	20.38
ATOM	2699	CE	LYS	A	391	20.072	29.882	47.532	1.00	24.61
ATOM	2700	NZ	LYS	A	391	21.393	30.332	48.051	1.00	26.71
ATOM	2701	N	GLU	A	392	14.824	30.849	44.682	1.00	22.91
ATOM	2702	CA	GLU	A	392	13.567	30.648	45.412	1.00	23.21
ATOM	2703	C	GLU	A	392	12.548	29.870	44.599	1.00	23.80
ATOM	2704	O	GLU	A	392	11.810	29.039	45.135	1.00	24.12
ATOM	2705	CB	GLU	A	392	12.926	31.967	45.854	1.00	23.58
ATOM	2706	CG	GLU	A	392	11.470	31.792	46.377	1.00	27.62
ATOM	2707	CD	GLU	A	392	11.219	32.416	47.762	1.00	30.72
ATOM	2708	OE1	GLU	A	392	12.080	33.184	48.243	1.00	34.21
ATOM	2709	OE2	GLU	A	392	10.157	32.158	48.370	1.00	30.26
ATOM	2710	N	LEU	A	393	12.436	30.212	43.322	1.00	22.69
ATOM	2711	CA	LEU	A	393	11.498	29.527	42.450	1.00	19.67

FIG. 2UU

ATOM	2712	C	LEU	A	393	11.862	28.036	42.415	1.00	16.28
ATOM	2713	O	LEU	A	393	11.010	27.163	42.580	1.00	16.68
ATOM	2714	CB	LEU	A	393	11.600	30.104	41.040	1.00	16.32
ATOM	2715	CG	LEU	A	393	10.942	31.443	40.796	1.00	11.54
ATOM	2716	CD1	LEU	A	393	11.522	32.077	39.540	1.00	11.13
ATOM	2717	CD2	LEU	A	393	9.453	31.217	40.635	1.00	12.66
ATOM	2718	N	ILE	A	394	13.148	27.771	42.261	1.00	14.10
ATOM	2719	CA	ILE	A	394	13.672	26.430	42.174	1.00	18.89
ATOM	2720	C	ILE	A	394	13.479	25.615	43.449	1.00	24.26
ATOM	2721	O	ILE	A	394	12.862	24.540	43.426	1.00	23.76
ATOM	2722	CB	ILE	A	394	15.140	26.499	41.738	1.00	17.71
ATOM	2723	CG1	ILE	A	394	15.191	26.982	40.280	1.00	17.72
ATOM	2724	CG2	ILE	A	394	15.835	25.173	41.915	1.00	20.38
ATOM	2725	CD1	ILE	A	394	16.539	26.785	39.598	1.00	17.90
ATOM	2726	N	TYR	A	395	13.974	26.145	44.567	1.00	26.90
ATOM	2727	CA	TYR	A	395	13.845	25.497	45.868	1.00	27.68
ATOM	2728	C	TYR	A	395	12.365	25.241	46.140	1.00	29.10
ATOM	2729	O	TYR	A	395	11.984	24.213	46.697	1.00	30.47
ATOM	2730	CB	TYR	A	395	14.426	26.414	46.943	1.00	26.11
ATOM	2731	CG	TYR	A	395	14.492	25.831	48.330	1.00	23.85
ATOM	2732	CD1	TYR	A	395	15.527	24.995	48.701	1.00	20.88
ATOM	2733	CD2	TYR	A	395	13.568	26.186	49.292	1.00	25.32
ATOM	2734	CE1	TYR	A	395	15.648	24.530	49.993	1.00	25.62
ATOM	2735	CE2	TYR	A	395	13.680	25.728	50.609	1.00	28.23
ATOM	2736	CZ	TYR	A	395	14.717	24.906	50.950	1.00	27.68
ATOM	2737	OH	TYR	A	395	14.814	24.469	52.245	1.00	33.57
ATOM	2738	N	LYS	A	396	11.524	26.166	45.697	1.00	31.19
ATOM	2739	CA	LYS	A	396	10.089	26.072	45.874	1.00	29.83
ATOM	2740	C	LYS	A	396	9.520	24.805	45.222	1.00	29.47
ATOM	2741	O	LYS	A	396	8.622	24.168	45.783	1.00	31.87
ATOM	2742	CB	LYS	A	396	9.451	27.297	45.236	1.00	31.22
ATOM	2743	CG	LYS	A	396	8.555	28.104	46.129	1.00	34.16
ATOM	2744	CD	LYS	A	396	9.323	28.880	47.193	1.00	36.62
ATOM	2745	CE	LYS	A	396	8.449	29.995	47.763	1.00	36.94
ATOM	2746	NZ	LYS	A	396	8.227	31.096	46.745	1.00	38.25
ATOM	2747	N	GLU	A	397	10.012	24.458	44.030	1.00	26.39
ATOM	2748	CA	GLU	A	397	9.524	23.280	43.308	1.00	23.47
ATOM	2749	C	GLU	A	397	10.077	21.984	43.863	1.00	19.67
ATOM	2750	O	GLU	A	397	9.398	20.968	43.869	1.00	18.33
ATOM	2751	CB	GLU	A	397	9.851	23.372	41.806	1.00	27.02
ATOM	2752	CG	GLU	A	397	8.703	23.869	40.887	1.00	27.93
ATOM	2753	CD	GLU	A	397	7.601	22.839	40.651	1.00	27.60
ATOM	2754	OE1	GLU	A	397	7.891	21.632	40.652	1.00	26.85
ATOM	2755	OE2	GLU	A	397	6.433	23.233	40.451	1.00	30.96
ATOM	2756	N	VAL	A	398	11.332	22.003	44.276	1.00	19.84
ATOM	2757	CA	VAL	A	398	11.966	20.822	44.833	1.00	23.53
ATOM	2758	C	VAL	A	398	11.255	20.413	46.119	1.00	26.29
ATOM	2759	O	VAL	A	398	11.114	19.217	46.400	1.00	29.23
ATOM	2760	CB	VAL	A	398	13.466	21.068	45.127	1.00	23.54
ATOM	2761	CG1	VAL	A	398	14.140	19.801	45.608	1.00	18.61
ATOM	2762	CG2	VAL	A	398	14.157	21.618	43.883	1.00	25.50
ATOM	2763	N	MET	A	399	10.789	21.404	46.884	1.00	28.85
ATOM	2764	CA	MET	A	399	10.081	21.137	48.135	1.00	31.54
ATOM	2765	C	MET	A	399	8.612	20.924	47.867	1.00	34.05
ATOM	2766	O	MET	A	399	7.892	20.478	48.753	1.00	36.36
ATOM	2767	CB	MET	A	399	10.242	22.287	49.129	1.00	29.76
ATOM	2768	CG	MET	A	399	11.666	22.576	49.515	1.00	32.50
ATOM	2769	SD	MET	A	399	12.612	21.136	50.101	1.00	34.26
ATOM	2770	CE	MET	A	399	12.505	21.419	51.848	1.00	42.05

FIG. 2VV

ATOM	2771	N	ASN A 400		8.185	21.209	46.636	1.00	38.05
ATOM	2772	CA	ASN A 400		6.782	21.075	46.197	1.00	42.57
ATOM	2773	C	ASN A 400		5.706	20.912	47.262	1.00	44.57
ATOM	2774	O	ASN A 400		4.935	21.885	47.424	1.00	46.32
ATOM	2775	CB	ASN A 400		6.585	20.032	45.047	1.00	44.49
ATOM	2776	CG	ASN A 400		7.320	18.689	45.274	1.00	46.24
ATOM	2777	OD1	ASN A 400		6.968	17.908	46.161	1.00	46.77
ATOM	2778	ND2	ASN A 400		8.289	18.390	44.401	1.00	44.05
ATOM	2779	C5	5184A1001		21.681	10.532	31.356	1.00	27.28
ATOM	2780	C6	5184A1001		22.457	11.213	30.225	1.00	28.05
ATOM	2781	O1	5184A1001		23.279	10.622	29.499	1.00	24.49
ATOM	2782	N1	5184A1001		22.218	12.549	30.129	1.00	26.81
ATOM	2783	C2	5184A1001		21.369	13.245	30.873	1.00	25.98
ATOM	2784	N3	5184A1001		20.662	12.674	31.791	1.00	28.30
ATOM	2785	C4	5184A1001		20.874	11.283	32.149	1.00	25.17
ATOM	2786	O2	5184A1001		21.212	14.442	30.751	1.00	28.54
ATOM	2787	C11	5184A1001		21.776	9.055	31.557	1.00	28.26
ATOM	2788	O4	5184A1001		21.021	8.534	32.380	1.00	29.45
ATOM	2789	N4	5184A1001		22.670	8.379	30.822	1.00	28.04
ATOM	2790	C1	5184A1001		23.707	4.452	30.694	1.00	24.51
ATOM	2791	C12	5184A1001		24.236	5.340	29.725	1.00	24.47
ATOM	2792	C3	5184A1001		23.837	6.674	29.834	1.00	25.42
ATOM	2793	C14	5184A1001		22.957	7.050	30.868	1.00	25.69
ATOM	2794	C7	5184A1001		22.454	6.120	31.816	1.00	25.22
ATOM	2795	C9	5184A1001		22.836	4.784	31.730	1.00	20.54
ATOM	2796	N2	5184A1001		20.058	10.764	33.215	1.00	24.72
ATOM	2797	C16	5184A1001		18.674	11.516	36.553	1.00	14.97
ATOM	2798	C13	5184A1001		19.542	11.079	35.546	1.00	19.43
ATOM	2799	C17	5184A1001		19.290	11.368	34.202	1.00	23.47
ATOM	2800	C15	5184A1001		18.143	12.127	33.889	1.00	25.12
ATOM	2801	C8	5184A1001		17.248	12.570	34.935	1.00	24.24
ATOM	2802	C10	5184A1001		17.543	12.248	36.274	1.00	15.35
ATOM	2803	OH2	TIP3B	1	19.519	6.665	33.090	1.00	11.81
ATOM	2804	OH2	TIP3B	2	14.148	22.210	28.179	1.00	20.00
ATOM	2805	OH2	TIP3B	3	16.487	15.191	32.609	1.00	20.00
					END				

FIG. 3A

Atom	Type	Resid	#	X	Y	Z	Occ	B
ATOM	1	CB	ASP	45	19.290	11.912	62.876	1.00	82.67
ATOM	2	CG	ASP	45	20.511	12.303	63.724	1.00	82.67
ATOM	3	OD1	ASP	45	21.632	12.419	63.162	1.00	82.67
ATOM	4	OD2	ASP	45	20.347	12.500	64.956	1.00	82.67
ATOM	5	C	ASP	45	19.675	12.871	60.534	1.00	40.50
ATOM	6	O	ASP	45	19.435	13.632	59.587	1.00	82.67
ATOM	7	N	ASP	45	17.424	12.934	61.581	1.00	40.50
ATOM	8	CA	ASP	45	18.894	13.005	61.859	1.00	40.50
ATOM	9	N	ASN	46	20.618	11.939	60.468	1.00	17.90
ATOM	10	CA	ASN	46	21.385	11.740	59.249	1.00	17.90
ATOM	11	CB	ASN	46	22.723	11.074	59.552	1.00	34.81
ATOM	12	CG	ASN	46	23.710	12.021	60.171	1.00	34.81
ATOM	13	OD1	ASN	46	23.339	13.104	60.639	1.00	34.81
ATOM	14	ND2	ASN	46	24.976	11.627	60.190	1.00	34.81
ATOM	15	C	ASN	46	20.650	10.894	58.227	1.00	17.90
ATOM	16	O	ASN	46	20.826	9.675	58.195	1.00	34.81
ATOM	17	N	GLN	47	19.813	11.534	57.410	1.00	2.36
ATOM	18	CA	GLN	47	19.079	10.827	56.360	1.00	2.36
ATOM	19	CB	GLN	47	17.776	11.552	55.999	1.00	25.20
ATOM	20	CG	GLN	47	16.591	11.308	56.965	1.00	25.20
ATOM	21	CD	GLN	47	15.309	12.062	56.565	1.00	25.20
ATOM	22	OE1	GLN	47	14.200	11.509	56.578	1.00	25.20
ATOM	23	NE2	GLN	47	15.462	13.338	56.226	1.00	25.20
ATOM	24	C	GLN	47	20.005	10.791	55.149	1.00	2.36
ATOM	25	O	GLN	47	19.903	9.907	54.306	1.00	25.20
ATOM	26	N	PHE	48	20.976	11.704	55.137	1.00	2.00
ATOM	27	CA	PHE	48	21.929	11.832	54.040	1.00	2.00
ATOM	28	CB	PHE	48	22.025	13.288	53.588	1.00	2.00
ATOM	29	CG	PHE	48	20.701	13.893	53.274	1.00	2.00
ATOM	30	CD1	PHE	48	19.915	14.404	54.296	1.00	2.00
ATOM	31	CD2	PHE	48	20.197	13.869	51.976	1.00	2.00
ATOM	32	CE1	PHE	48	18.638	14.876	54.054	1.00	2.00
ATOM	33	CE2	PHE	48	18.918	14.337	51.707	1.00	2.00
ATOM	34	CZ	PHE	48	18.128	14.845	52.760	1.00	2.00
ATOM	35	C	PHE	48	23.314	11.359	54.369	1.00	2.00
ATOM	36	O	PHE	48	23.672	11.164	55.529	1.00	2.00
ATOM	37	N	TYR	49	24.098	11.171	53.320	1.00	2.00
ATOM	38	CA	TYR	49	25.465	10.754	53.478	1.00	2.00
ATOM	39	CB	TYR	49	25.572	9.230	53.557	1.00	7.42
ATOM	40	CG	TYR	49	25.519	8.504	52.242	1.00	7.42
ATOM	41	CD1	TYR	49	24.305	8.195	51.643	1.00	7.42
ATOM	42	CE1	TYR	49	24.255	7.486	50.442	1.00	7.42
ATOM	43	CD2	TYR	49	26.684	8.085	51.619	1.00	7.42
ATOM	44	CE2	TYR	49	26.641	7.380	50.416	1.00	7.42
ATOM	45	CZ	TYR	49	25.426	7.084	49.841	1.00	7.42
ATOM	46	OH	TYR	49	25.387	6.407	48.655	1.00	7.42
ATOM	47	C	TYR	49	26.250	11.304	52.311	1.00	2.00
ATOM	48	O	TYR	49	25.746	11.416	51.202	1.00	7.42
ATOM	49	N	SER	50	27.484	11.681	52.585	1.00	12.70
ATOM	50	CA	SER	50	28.346	12.240	51.569	1.00	12.70
ATOM	51	CB	SER	50	29.144	13.410	52.158	1.00	44.73
ATOM	52	OG	SER	50	28.278	14.435	52.609	1.00	44.73
ATOM	53	C	SER	50	29.303	11.208	51.002	1.00	12.70
ATOM	54	O	SER	50	29.989	10.507	51.744	1.00	44.73
ATOM	55	N	VAL	51	29.343	11.127	49.676	1.00	12.81
ATOM	56	CA	VAL	51	30.238	10.209	48.993	1.00	12.81
ATOM	57	CB	VAL	51	29.531	8.902	48.549	1.00	2.00

FIG. 3B

ATOM	58	CG1	VAL	51	28.521	9.154	47.453	1.00	2.00
ATOM	59	CG2	VAL	51	30.557	7.887	48.125	1.00	2.00
ATOM	60	C	VAL	51	30.898	10.933	47.828	1.00	12.81
ATOM	61	O	VAL	51	30.242	11.660	47.076	1.00	2.00
ATOM	62	N	GLU	52	32.222	10.801	47.753	1.00	26.73
ATOM	63	CA	GLU	52	33.013	11.448	46.709	1.00	26.73
ATOM	64	CB	GLU	52	34.479	11.575	47.151	1.00	23.83
ATOM	65	CG	GLU	52	35.286	12.607	46.355	1.00	23.83
ATOM	66	CD	GLU	52	34.838	14.037	46.631	1.00	23.83
ATOM	67	OE1	GLU	52	34.719	14.388	47.824	1.00	23.83
ATOM	68	OE2	GLU	52	34.605	14.804	45.666	1.00	23.83
ATOM	69	C	GLU	52	32.921	10.677	45.388	1.00	26.73
ATOM	70	O	GLU	52	33.710	9.760	45.127	1.00	23.83
ATOM	71	N	VAL	53	31.948	11.054	44.562	1.00	31.39
ATOM	72	CA	VAL	53	31.741	10.409	43.266	1.00	31.39
ATOM	73	CB	VAL	53	30.228	10.287	42.885	1.00	19.10
ATOM	74	CG1	VAL	53	30.072	9.701	41.480	1.00	19.10
ATOM	75	CG2	VAL	53	29.496	9.401	43.878	1.00	19.10
ATOM	76	C	VAL	53	32.471	11.190	42.175	1.00	31.39
ATOM	77	O	VAL	53	32.073	12.305	41.814	1.00	19.10
ATOM	78	N	GLY	54	33.554	10.603	41.670	1.00	28.22
ATOM	79	CA	GLY	54	34.329	11.234	40.617	1.00	28.22
ATOM	80	C	GLY	54	35.125	12.430	41.089	1.00	28.22
ATOM	81	O	GLY	54	36.150	12.291	41.758	1.00	37.37
ATOM	82	N	ASP	55	34.617	13.611	40.767	1.00	24.29
ATOM	83	CA	ASP	55	35.257	14.881	41.106	1.00	24.29
ATOM	84	CB	ASP	55	35.557	15.616	39.784	1.00	45.10
ATOM	85	CG	ASP	55	36.481	16.802	39.952	1.00	45.10
ATOM	86	OD1	ASP	55	37.585	16.632	40.524	1.00	45.10
ATOM	87	OD2	ASP	55	36.110	17.895	39.466	1.00	45.10
ATOM	88	C	ASP	55	34.317	15.730	41.969	1.00	24.29
ATOM	89	O	ASP	55	34.669	16.829	42.404	1.00	45.10
ATOM	90	N	SER	56	33.126	15.193	42.214	1.00	28.43
ATOM	91	CA	SER	56	32.089	15.876	42.974	1.00	28.43
ATOM	92	CB	SER	56	30.865	16.086	42.060	1.00	50.26
ATOM	93	OG	SER	56	30.177	17.303	42.334	1.00	50.26
ATOM	94	C	SER	56	31.686	15.067	44.207	1.00	28.43
ATOM	95	O	SER	56	31.861	13.852	44.254	1.00	50.26
ATOM	96	N	THR	57	31.159	15.751	45.213	1.00	21.09
ATOM	97	CA	THR	57	30.724	15.085	46.428	1.00	21.09
ATOM	98	CB	THR	57	31.153	15.856	47.683	1.00	27.49
ATOM	99	OG1	THR	57	32.532	16.234	47.561	1.00	27.49
ATOM	100	CG2	THR	57	30.967	14.991	48.931	1.00	27.49
ATOM	101	C	THR	57	29.208	14.955	46.444	1.00	21.09
ATOM	102	O	THR	57	28.498	15.934	46.680	1.00	27.49
ATOM	103	N	PHE	58	28.721	13.749	46.173	1.00	33.68
ATOM	104	CA	PHE	58	27.290	13.494	46.171	1.00	33.68
ATOM	105	CB	PHE	58	26.942	12.309	45.281	1.00	8.44
ATOM	106	CG	PHE	58	26.690	12.677	43.841	1.00	8.44
ATOM	107	CD1	PHE	58	27.731	13.123	43.030	1.00	8.44
ATOM	108	CD2	PHE	58	25.425	12.514	43.286	1.00	8.44
ATOM	109	CE1	PHE	58	27.526	13.382	41.671	1.00	8.44
ATOM	110	CE2	PHE	58	25.198	12.765	41.930	1.00	8.44
ATOM	111	CZ	PHE	58	26.252	13.207	41.119	1.00	8.44
ATOM	112	C	PHE	58	26.790	13.230	47.584	1.00	33.68
ATOM	113	O	PHE	58	27.306	12.360	48.283	1.00	8.44
ATOM	114	N	THR	59	25.836	14.045	48.017	1.00	2.00
ATOM	115	CA	THR	59	25.235	13.913	49.331	1.00	2.00
ATOM	116	CB	THR	59	25.238	15.234	50.117	1.00	2.11

FIG. 3C

ATOM	117	OG1	THR	59	26.579	15.724	50.239	1.00	2.11
ATOM	118	CG2	THR	59	24.658	15.016	51.488	1.00	2.11
ATOM	119	C	THR	59	23.803	13.478	49.095	1.00	2.00
ATOM	120	O	THR	59	22.910	14.290	48.899	1.00	2.11
ATOM	121	N	VAL	60	23.598	12.174	49.091	1.00	16.21
ATOM	122	CA	VAL	60	22.281	11.629	48.857	1.00	16.21
ATOM	123	CB	VAL	60	22.316	10.642	47.669	1.00	12.96
ATOM	124	CG1	VAL	60	22.576	11.384	46.380	1.00	12.96
ATOM	125	CG2	VAL	60	23.409	9.597	47.883	1.00	12.96
ATOM	126	C	VAL	60	21.700	10.933	50.078	1.00	16.21
ATOM	127	O	VAL	60	22.367	10.773	51.098	1.00	12.96
ATOM	128	N	LEU	61	20.423	10.577	49.964	1.00	2.00
ATOM	129	CA	LEU	61	19.689	9.868	51.001	1.00	2.00
ATOM	130	CB	LEU	61	18.228	9.724	50.591	1.00	19.79
ATOM	131	CG	LEU	61	17.323	10.947	50.539	1.00	19.79
ATOM	132	CD1	LEU	61	16.195	10.678	49.580	1.00	19.79
ATOM	133	CD2	LEU	61	16.787	11.243	51.919	1.00	19.79
ATOM	134	C	LEU	61	20.271	8.471	51.136	1.00	2.00
ATOM	135	O	LEU	61	20.721	7.889	50.163	1.00	19.79
ATOM	136	N	LYS	62	20.179	7.903	52.328	1.00	37.57
ATOM	137	CA	LYS	62	20.713	6.567	52.597	1.00	37.57
ATOM	138	CB	LYS	62	20.514	6.215	54.080	1.00	12.42
ATOM	139	CG	LYS	62	21.129	7.196	55.073	1.00	12.42
ATOM	140	CD	LYS	62	22.637	7.031	55.239	1.00	12.42
ATOM	141	CE	LYS	62	23.193	8.033	56.258	1.00	12.42
ATOM	142	NZ	LYS	62	22.571	7.914	57.624	1.00	12.42
ATOM	143	C	LYS	62	20.184	5.431	51.708	1.00	37.57
ATOM	144	O	LYS	62	20.898	4.467	51.448	1.00	12.42
ATOM	145	N	ARG	63	18.942	5.543	51.250	1.00	5.93
ATOM	146	CA	ARG	63	18.334	4.516	50.406	1.00	5.93
ATOM	147	CB	ARG	63	16.890	4.912	50.057	1.00	2.00
ATOM	148	CG	ARG	63	16.779	6.198	49.253	1.00	2.00
ATOM	149	CD	ARG	63	15.381	6.764	49.236	1.00	2.00
ATOM	150	NE	ARG	63	14.458	5.942	48.467	1.00	2.00
ATOM	151	CZ	ARG	63	13.205	6.281	48.192	1.00	2.00
ATOM	152	NH1	ARG	63	12.718	7.423	48.625	1.00	2.00
ATOM	153	NH2	ARG	63	12.428	5.465	47.500	1.00	2.00
ATOM	154	C	ARG	63	19.140	4.295	49.129	1.00	5.93
ATOM	155	O	ARG	63	19.239	3.168	48.640	1.00	2.00
ATOM	156	N	TYR	64	19.715	5.384	48.615	1.00	12.13
ATOM	157	CA	TYR	64	20.516	5.377	47.391	1.00	12.13
ATOM	158	CB	TYR	64	20.460	6.764	46.721	1.00	2.00
ATOM	159	CG	TYR	64	19.066	7.169	46.288	1.00	2.00
ATOM	160	CD1	TYR	64	18.358	6.407	45.361	1.00	2.00
ATOM	161	CE1	TYR	64	17.052	6.724	45.011	1.00	2.00
ATOM	162	CD2	TYR	64	18.422	8.275	46.844	1.00	2.00
ATOM	163	CE2	TYR	64	17.109	8.599	46.487	1.00	2.00
ATOM	164	CZ	TYR	64	16.432	7.810	45.571	1.00	2.00
ATOM	165	OH	TYR	64	15.118	8.058	45.230	1.00	2.00
ATOM	166	C	TYR	64	21.951	4.968	47.710	1.00	12.13
ATOM	167	O	TYR	64	22.691	5.711	48.360	1.00	2.00
ATOM	168	N	GLN	65	22.349	3.791	47.242	1.00	2.00
ATOM	169	CA	GLN	65	23.675	3.299	47.538	1.00	2.00
ATOM	170	CB	GLN	65	23.582	2.235	48.631	1.00	32.87
ATOM	171	CG	GLN	65	22.537	1.153	48.353	1.00	32.87
ATOM	172	CD	GLN	65	21.813	0.677	49.618	1.00	32.87
ATOM	173	OE1	GLN	65	21.091	1.448	50.266	1.00	32.87
ATOM	174	NE2	GLN	65	21.990	-0.598	49.963	1.00	32.87
ATOM	175	C	GLN	65	24.468	2.770	46.347	1.00	2.00

FIG. 3D

ATOM	176	O	GLN	65	23.912	2.442	45.298	1.00	32.87
ATOM	177	N	ASN	66	25.783	2.677	46.550	1.00	28.78
ATOM	178	CA	ASN	66	26.745	2.207	45.561	1.00	28.78
ATOM	179	CB	ASN	66	26.528	0.746	45.218	1.00	23.20
ATOM	180	CG	ASN	66	27.649	0.186	44.374	1.00	23.20
ATOM	181	OD1	ASN	66	27.409	-0.590	43.449	1.00	23.20
ATOM	182	ND2	ASN	66	28.879	0.591	44.668	1.00	23.20
ATOM	183	C	ASN	66	26.680	3.054	44.319	1.00	28.78
ATOM	184	O	ASN	66	26.403	2.566	43.225	1.00	23.20
ATOM	185	N	LEU	67	26.961	4.335	44.514	1.00	28.28
ATOM	186	CA	LEU	67	26.928	5.310	43.442	1.00	28.28
ATOM	187	CB	LEU	67	27.105	6.717	44.014	1.00	5.06
ATOM	188	CG	LEU	67	26.056	7.332	44.932	1.00	5.06
ATOM	189	CD1	LEU	67	25.803	8.741	44.446	1.00	5.06
ATOM	190	CD2	LEU	67	24.758	6.538	44.949	1.00	5.06
ATOM	191	C	LEU	67	28.000	5.065	42.389	1.00	28.28
ATOM	192	O	LEU	67	29.169	4.878	42.717	1.00	5.06
ATOM	193	N	LYS	68	27.584	4.986	41.134	1.00	4.06
ATOM	194	CA	LYS	68	28.520	4.828	40.029	1.00	4.06
ATOM	195	CB	LYS	68	28.249	3.541	39.233	1.00	30.89
ATOM	196	CG	LYS	68	28.684	2.239	39.906	1.00	30.89
ATOM	197	CD	LYS	68	27.651	1.114	39.714	1.00	30.89
ATOM	198	CE	LYS	68	27.352	0.852	38.225	1.00	30.89
ATOM	199	NZ	LYS	68	26.455	-0.335	37.986	1.00	30.89
ATOM	200	C	LYS	68	28.269	6.044	39.143	1.00	4.06
ATOM	201	O	LYS	68	27.130	6.316	38.761	1.00	30.89
ATOM	202	N	PRO	69	29.319	6.841	38.874	1.00	44.94
ATOM	203	CD	PRO	69	30.714	6.698	39.337	1.00	33.19
ATOM	204	CA	PRO	69	29.156	8.027	38.023	1.00	44.94
ATOM	205	CB	PRO	69	30.492	8.752	38.196	1.00	33.19
ATOM	206	CG	PRO	69	31.475	7.618	38.394	1.00	33.19
ATOM	207	C	PRO	69	28.925	7.587	36.576	1.00	44.94
ATOM	208	O	PRO	69	29.574	6.657	36.090	1.00	33.19
ATOM	209	N	ILE	70	27.943	8.198	35.922	1.00	11.68
ATOM	210	CA	ILE	70	27.612	7.848	34.544	1.00	11.68
ATOM	211	CB	ILE	70	26.421	6.854	34.506	1.00	15.82
ATOM	212	CG2	ILE	70	26.794	5.535	35.192	1.00	15.82
ATOM	213	CG1	ILE	70	25.222	7.453	35.236	1.00	15.82
ATOM	214	CD1	ILE	70	23.924	6.747	34.955	1.00	15.82
ATOM	215	C	ILE	70	27.230	9.078	33.713	1.00	11.68
ATOM	216	O	ILE	70	26.365	8.989	32.837	1.00	15.82
ATOM	217	N	GLY	71	27.884	10.214	33.959	1.00	53.07
ATOM	218	CA	GLY	71	27.544	11.425	33.218	1.00	53.07
ATOM	219	C	GLY	71	28.586	12.527	33.070	1.00	53.07
ATOM	220	O	GLY	71	29.419	12.471	32.147	1.00	47.75
ATOM	221	N	SER	72	28.502	13.543	33.938	1.00	33.54
ATOM	222	CA	SER	72	29.400	14.711	33.924	1.00	33.54
ATOM	223	CB	SER	72	30.878	14.285	33.938	1.00	47.06
ATOM	224	OG	SER	72	31.592	14.895	34.997	1.00	47.06
ATOM	225	C	SER	72	29.135	15.607	32.716	1.00	33.54
ATOM	226	O	SER	72	28.349	16.563	32.873	1.00	47.06
ATOM	227	CB	ILE	77	27.336	15.379	37.733	1.00	14.51
ATOM	228	CG2	ILE	77	28.188	14.104	37.638	1.00	14.51
ATOM	229	CG1	ILE	77	28.142	16.653	37.434	1.00	14.51
ATOM	230	CD1	ILE	77	29.294	16.914	38.389	1.00	14.51
ATOM	231	C	ILE	77	25.290	14.058	37.115	1.00	32.22
ATOM	232	O	ILE	77	24.717	13.978	38.207	1.00	14.51
ATOM	233	N	ILE	77	25.299	16.530	36.838	1.00	32.22
ATOM	234	CA	ILE	77	26.134	15.291	36.771	1.00	32.22

FIG. 3E

ATOM	235	N	VAL	78	25.197	13.114	36.177	1.00	2.00
ATOM	236	CA	VAL	78	24.407	11.907	36.396	1.00	2.00
ATOM	237	CB	VAL	78	23.839	11.313	35.083	1.00	6.06
ATOM	238	CG1	VAL	78	22.756	10.284	35.408	1.00	6.06
ATOM	239	CG2	VAL	78	23.279	12.411	34.177	1.00	6.06
ATOM	240	C	VAL	78	25.198	10.845	37.133	1.00	2.00
ATOM	241	O	VAL	78	26.419	10.736	36.983	1.00	6.06
ATOM	242	N	CYS	79	24.484	10.048	37.918	1.00	14.03
ATOM	243	CA	CYS	79	25.112	9.016	38.713	1.00	14.03
ATOM	244	CB	CYS	79	25.565	9.636	40.024	1.00	23.50
ATOM	245	SG	CYS	79	26.799	8.691	40.861	1.00	23.50
ATOM	246	C	CYS	79	24.178	7.836	38.975	1.00	14.03
ATOM	247	O	CYS	79	23.128	7.996	39.581	1.00	23.50
ATOM	248	N	ALA	80	24.578	6.649	38.524	1.00	14.88
ATOM	249	CA	ALA	80	23.782	5.438	38.707	1.00	14.88
ATOM	250	CB	ALA	80	24.281	4.360	37.783	1.00	19.57
ATOM	251	C	ALA	80	23.831	4.956	40.147	1.00	14.88
ATOM	252	O	ALA	80	24.850	5.100	40.820	1.00	19.57
ATOM	253	N	ALA	81	22.728	4.401	40.634	1.00	5.14
ATOM	254	CA	ALA	81	22.703	3.909	42.005	1.00	5.14
ATOM	255	CB	ALA	81	22.560	5.055	42.962	1.00	20.04
ATOM	256	C	ALA	81	21.593	2.916	42.246	1.00	5.14
ATOM	257	O	ALA	81	20.689	2.771	41.425	1.00	20.04
ATOM	258	N	TYR	82	21.676	2.227	43.382	1.00	10.44
ATOM	259	CA	TYR	82	20.672	1.251	43.787	1.00	10.44
ATOM	260	CB	TYR	82	21.365	0.005	44.330	1.00	17.29
ATOM	261	CG	TYR	82	20.477	-0.907	45.132	1.00	17.29
ATOM	262	CD1	TYR	82	19.335	-1.475	44.572	1.00	17.29
ATOM	263	CE1	TYR	82	18.509	-2.330	45.311	1.00	17.29
ATOM	264	CD2	TYR	82	20.780	-1.212	46.450	1.00	17.29
ATOM	265	CE2	TYR	82	19.964	-2.069	47.197	1.00	17.29
ATOM	266	CZ	TYR	82	18.832	-2.623	46.619	1.00	17.29
ATOM	267	OH	TYR	82	18.049	-3.479	47.351	1.00	17.29
ATOM	268	C	TYR	82	19.763	1.830	44.861	1.00	10.44
ATOM	269	O	TYR	82	20.246	2.290	45.885	1.00	17.29
ATOM	270	N	ASP	83	18.457	1.830	44.623	1.00	5.91
ATOM	271	CA	ASP	83	17.525	2.325	45.624	1.00	5.91
ATOM	272	CB	ASP	83	16.299	2.969	44.989	1.00	26.75
ATOM	273	CG	ASP	83	15.358	3.573	46.021	1.00	26.75
ATOM	274	OD1	ASP	83	15.707	3.588	47.211	1.00	26.75
ATOM	275	OD2	ASP	83	14.269	4.050	45.656	1.00	26.75
ATOM	276	C	ASP	83	17.088	1.131	46.466	1.00	5.91
ATOM	277	O	ASP	83	16.418	0.217	45.972	1.00	26.75
ATOM	278	N	ALA	84	17.415	1.181	47.755	1.00	3.12
ATOM	279	CA	ALA	84	17.099	0.113	48.680	1.00	3.12
ATOM	280	CB	ALA	84	17.949	0.249	49.920	1.00	15.64
ATOM	281	C	ALA	84	15.626	0.049	49.043	1.00	3.12
ATOM	282	O	ALA	84	15.123	-1.025	49.355	1.00	15.64
ATOM	283	N	VAL	85	14.923	1.176	48.979	1.00	2.05
ATOM	284	CA	VAL	85	13.503	1.203	49.320	1.00	2.05
ATOM	285	CB	VAL	85	13.012	2.652	49.634	1.00	2.17
ATOM	286	CG1	VAL	85	11.487	2.690	49.830	1.00	2.17
ATOM	287	CG2	VAL	85	13.718	3.172	50.883	1.00	2.17
ATOM	288	C	VAL	85	12.625	0.586	48.243	1.00	2.05
ATOM	289	O	VAL	85	11.834	-0.321	48.510	1.00	2.17
ATOM	290	N	LEU	86	12.784	1.094	47.026	1.00	6.01
ATOM	291	CA	LEU	86	12.030	0.649	45.859	1.00	6.01
ATOM	292	CB	LEU	86	12.116	1.726	44.784	1.00	19.18
ATOM	293	CG	LEU	86	10.838	2.271	44.158	1.00	19.18

FIG. 3F

ATOM	294	CD1	LEU	86	9.901	2.763	45.248	1.00	19.18
ATOM	295	CD2	LEU	86	11.203	3.392	43.186	1.00	19.18
ATOM	296	C	LEU	86	12.585	-0.655	45.307	1.00	6.01
ATOM	297	O	LEU	86	11.890	-1.369	44.591	1.00	19.18
ATOM	298	N	ASP	87	13.837	-0.948	45.649	1.00	2.44
ATOM	299	CA	ASP	87	14.539	-2.147	45.199	1.00	2.44
ATOM	300	CB	ASP	87	13.928	-3.445	45.782	1.00	23.73
ATOM	301	CG	ASP	87	14.691	-4.710	45.341	1.00	23.73
ATOM	302	OD1	ASP	87	15.932	-4.794	45.560	1.00	23.73
ATOM	303	OD2	ASP	87	14.045	-5.612	44.751	1.00	23.73
ATOM	304	C	ASP	87	14.650	-2.228	43.674	1.00	2.44
ATOM	305	O	ASP	87	14.020	-3.071	43.017	1.00	23.73
ATOM	306	N	ARG	88	15.468	-1.339	43.130	1.00	6.10
ATOM	307	CA	ARG	88	15.734	-1.260	41.700	1.00	6.10
ATOM	308	CB	ARG	88	14.490	-0.823	40.902	1.00	16.86
ATOM	309	CG	ARG	88	13.796	0.433	41.398	1.00	16.86
ATOM	310	CD	ARG	88	12.410	0.571	40.797	1.00	16.86
ATOM	311	NE	ARG	88	12.349	1.547	39.706	1.00	16.86
ATOM	312	CZ	ARG	88	11.238	2.182	39.327	1.00	16.86
ATOM	313	NH1	ARG	88	10.089	1.943	39.956	1.00	16.86
ATOM	314	NH2	ARG	88	11.263	3.057	38.326	1.00	16.86
ATOM	315	C	ARG	88	16.845	-0.258	41.537	1.00	6.10
ATOM	316	O	ARG	88	17.301	0.340	42.512	1.00	16.86
ATOM	317	N	ASN	89	17.315	-0.100	40.311	1.00	21.92
ATOM	318	CA	ASN	89	18.378	0.848	40.067	1.00	21.92
ATOM	319	CB	ASN	89	19.448	0.232	39.178	1.00	6.92
ATOM	320	CG	ASN	89	20.210	-0.864	39.884	1.00	6.92
ATOM	321	OD1	ASN	89	21.057	-0.588	40.718	1.00	6.92
ATOM	322	ND2	ASN	89	19.891	-2.114	39.578	1.00	6.92
ATOM	323	C	ASN	89	17.821	2.144	39.510	1.00	21.92
ATOM	324	O	ASN	89	16.824	2.156	38.782	1.00	6.92
ATOM	325	N	VAL	90	18.433	3.237	39.950	1.00	2.00
ATOM	326	CA	VAL	90	18.044	4.579	39.567	1.00	2.00
ATOM	327	CB	VAL	90	17.273	5.295	40.721	1.00	2.00
ATOM	328	CG1	VAL	90	15.944	4.612	40.995	1.00	2.00
ATOM	329	CG2	VAL	90	18.112	5.324	41.985	1.00	2.00
ATOM	330	C	VAL	90	19.246	5.441	39.153	1.00	2.00
ATOM	331	O	VAL	90	20.409	5.041	39.299	1.00	2.00
ATOM	332	N	ALA	91	18.935	6.609	38.590	1.00	2.00
ATOM	333	CA	ALA	91	19.920	7.584	38.140	1.00	2.00
ATOM	334	CB	ALA	91	19.749	7.871	36.659	1.00	2.00
ATOM	335	C	ALA	91	19.680	8.844	38.952	1.00	2.00
ATOM	336	O	ALA	91	18.565	9.335	39.027	1.00	2.00
ATOM	337	N	ILE	92	20.731	9.343	39.583	1.00	12.92
ATOM	338	CA	ILE	92	20.646	10.544	40.401	1.00	12.92
ATOM	339	CB	ILE	92	21.263	10.298	41.817	1.00	2.00
ATOM	340	CG2	ILE	92	21.166	11.566	42.671	1.00	2.00
ATOM	341	CG1	ILE	92	20.583	9.100	42.502	1.00	2.00
ATOM	342	CD1	ILE	92	21.274	8.619	43.742	1.00	2.00
ATOM	343	C	ILE	92	21.397	11.673	39.702	1.00	12.92
ATOM	344	O	ILE	92	22.570	11.534	39.361	1.00	2.00
ATOM	345	N	LYS	93	20.726	12.803	39.539	1.00	9.99
ATOM	346	CA	LYS	93	21.313	13.946	38.870	1.00	9.99
ATOM	347	CB	LYS	93	20.419	14.349	37.697	1.00	19.91
ATOM	348	CG	LYS	93	20.968	15.445	36.831	1.00	19.91
ATOM	349	CD	LYS	93	19.986	15.786	35.748	1.00	19.91
ATOM	350	CE	LYS	93	20.615	16.681	34.704	1.00	19.91
ATOM	351	NZ	LYS	93	19.611	16.999	33.658	1.00	19.91
ATOM	352	C	LYS	93	21.506	15.130	39.817	1.00	9.99

FIG. 3G

ATOM	353	O	LYS	93	20.538	15.702	40.322	1.00	19.91
ATOM	354	N	LYS	94	22.763	15.491	40.056	1.00	7.04
ATOM	355	CA	LYS	94	23.086	16.609	40.931	1.00	7.04
ATOM	356	CB	LYS	94	24.434	16.381	41.605	1.00	2.00
ATOM	357	CG	LYS	94	24.823	17.501	42.548	1.00	2.00
ATOM	358	CD	LYS	94	26.242	17.356	43.019	1.00	2.00
ATOM	359	CE	LYS	94	26.594	18.461	43.976	1.00	2.00
ATOM	360	NZ	LYS	94	27.975	18.303	44.477	1.00	2.00
ATOM	361	C	LYS	94	23.138	17.944	40.191	1.00	7.04
ATOM	362	O	LYS	94	24.036	18.167	39.374	1.00	2.00
ATOM	363	N	LEU	95	22.197	18.834	40.503	1.00	2.00
ATOM	364	CA	LEU	95	22.129	20.168	39.913	1.00	2.00
ATOM	365	CB	LEU	95	20.664	20.608	39.757	1.00	2.18
ATOM	366	CG	LEU	95	19.934	20.373	38.438	1.00	2.18
ATOM	367	CD1	LEU	95	20.243	19.003	37.867	1.00	2.18
ATOM	368	CD2	LEU	95	18.445	20.557	38.649	1.00	2.18
ATOM	369	C	LEU	95	22.863	21.150	40.829	1.00	2.00
ATOM	370	O	LEU	95	22.262	21.753	41.717	1.00	2.18
ATOM	371	N	SER	96	24.168	21.305	40.606	1.00	21.89
ATOM	372	CA	SER	96	25.009	22.206	41.414	1.00	21.89
ATOM	373	CB	SER	96	26.497	21.998	41.101	1.00	46.05
ATOM	374	OG	SER	96	26.868	20.628	41.129	1.00	46.05
ATOM	375	C	SER	96	24.675	23.679	41.215	1.00	21.89
ATOM	376	O	SER	96	24.844	24.223	40.122	1.00	46.05
ATOM	377	N	ARG	97	24.166	24.312	42.266	1.00	23.50
ATOM	378	CA	ARG	97	23.831	25.734	42.214	1.00	23.50
ATOM	379	CB	ARG	97	25.128	26.553	42.134	1.00	38.04
ATOM	380	CG	ARG	97	25.891	26.663	43.424	1.00	38.04
ATOM	381	CD	ARG	97	25.228	27.665	44.345	1.00	38.04
ATOM	382	NE	ARG	97	26.077	27.967	45.493	1.00	38.04
ATOM	383	CZ	ARG	97	25.800	28.884	46.422	1.00	38.04
ATOM	384	NH1	ARG	97	24.686	29.619	46.351	1.00	38.04
ATOM	385	NH2	ARG	97	26.643	29.058	47.439	1.00	38.04
ATOM	386	C	ARG	97	22.964	26.037	40.991	1.00	23.50
ATOM	387	O	ARG	97	23.340	26.838	40.150	1.00	38.04
ATOM	388	N	PRO	98	21.798	25.384	40.871	1.00	46.09
ATOM	389	CD	PRO	98	21.195	24.520	41.896	1.00	35.22
ATOM	390	CA	PRO	98	20.873	25.573	39.736	1.00	46.09
ATOM	391	CB	PRO	98	19.630	24.787	40.166	1.00	35.22
ATOM	392	CG	PRO	98	19.723	24.759	41.683	1.00	35.22
ATOM	393	C	PRO	98	20.528	27.027	39.400	1.00	46.09
ATOM	394	O	PRO	98	20.320	27.376	38.228	1.00	35.22
ATOM	395	N	PHE	99	20.507	27.865	40.430	1.00	24.90
ATOM	396	CA	PHE	99	20.192	29.286	40.306	1.00	24.90
ATOM	397	CB	PHE	99	19.490	29.740	41.585	1.00	11.96
ATOM	398	CG	PHE	99	20.122	29.194	42.831	1.00	11.96
ATOM	399	CD1	PHE	99	21.164	29.879	43.454	1.00	11.96
ATOM	400	CD2	PHE	99	19.724	27.964	43.338	1.00	11.96
ATOM	401	CE1	PHE	99	21.804	29.348	44.556	1.00	11.96
ATOM	402	CE2	PHE	99	20.353	27.418	44.439	1.00	11.96
ATOM	403	CZ	PHE	99	21.401	28.108	45.053	1.00	11.96
ATOM	404	C	PHE	99	21.420	30.169	40.058	1.00	24.90
ATOM	405	O	PHE	99	21.334	31.381	40.173	1.00	11.96
ATOM	406	N	GLN	100	22.555	29.588	39.695	1.00	11.02
ATOM	407	CA	GLN	100	23.751	30.394	39.462	1.00	11.02
ATOM	408	CB	GLN	100	24.942	29.520	39.089	1.00	30.87
ATOM	409	CG	GLN	100	24.666	28.644	37.920	1.00	30.87
ATOM	410	CD	GLN	100	25.797	27.707	37.635	1.00	30.87
ATOM	411	OE1	GLN	100	26.602	27.945	36.736	1.00	30.87

FIG. 3H

ATOM	412	NE2	GLN	100	25.870	26.622	38.399	1.00	30.87
ATOM	413	C	GLN	100	23.531	31.470	38.397	1.00	11.02
ATOM	414	O	GLN	100	24.109	32.553	38.495	1.00	30.87
ATOM	415	N	ASN	101	22.746	31.144	37.363	1.00	17.49
ATOM	416	CA	ASN	101	22.414	32.077	36.288	1.00	17.49
ATOM	417	CB	ASN	101	23.525	32.176	35.220	1.00	4.38
ATOM	418	CG	ASN	101	24.074	30.827	34.774	1.00	4.38
ATOM	419	OD1	ASN	101	23.393	30.060	34.095	1.00	4.38
ATOM	420	ND2	ASN	101	25.337	30.564	35.100	1.00	4.38
ATOM	421	C	ASN	101	21.044	31.739	35.699	1.00	17.49
ATOM	422	O	ASN	101	20.607	30.602	35.759	1.00	4.38
ATOM	423	N	GLN	102	20.363	32.750	35.167	1.00	9.50
ATOM	424	CA	GLN	102	19.019	32.597	34.603	1.00	9.50
ATOM	425	CB	GLN	102	18.500	33.916	34.018	1.00	10.21
ATOM	426	CG	GLN	102	18.213	35.035	34.991	1.00	10.21
ATOM	427	CD	GLN	102	17.250	36.039	34.397	1.00	10.21
ATOM	428	OE1	GLN	102	16.111	35.689	34.091	1.00	10.21
ATOM	429	NE2	GLN	102	17.699	37.288	34.210	1.00	10.21
ATOM	430	C	GLN	102	18.886	31.546	33.531	1.00	9.50
ATOM	431	O	GLN	102	17.784	31.107	33.256	1.00	10.21
ATOM	432	N	THR	103	19.978	31.228	32.844	1.00	2.00
ATOM	433	CA	THR	103	19.922	30.202	31.812	1.00	2.00
ATOM	434	CB	THR	103	21.194	30.227	30.920	1.00	25.55
ATOM	435	OG1	THR	103	21.433	31.565	30.460	1.00	25.55
ATOM	436	CG2	THR	103	21.022	29.327	29.693	1.00	25.55
ATOM	437	C	THR	103	19.754	28.863	32.538	1.00	2.00
ATOM	438	O	THR	103	18.848	28.088	32.232	1.00	25.55
ATOM	439	N	HIS	104	20.574	28.656	33.570	1.00	2.12
ATOM	440	CA	HIS	104	20.525	27.455	34.412	1.00	2.12
ATOM	441	CB	HIS	104	21.704	27.415	35.382	1.00	27.31
ATOM	442	CG	HIS	104	22.953	26.854	34.794	1.00	27.31
ATOM	443	CD2	HIS	104	23.166	25.754	34.034	1.00	27.31
ATOM	444	ND1	HIS	104	24.186	27.434	34.984	1.00	27.31
ATOM	445	CE1	HIS	104	25.109	26.712	34.373	1.00	27.31
ATOM	446	NE2	HIS	104	24.513	25.687	33.788	1.00	27.31
ATOM	447	C	HIS	104	19.252	27.426	35.231	1.00	2.12
ATOM	448	O	HIS	104	18.685	26.371	35.460	1.00	27.31
ATOM	449	N	ALA	105	18.812	28.590	35.669	1.00	2.00
ATOM	450	CA	ALA	105	17.626	28.687	36.482	1.00	2.00
ATOM	451	CB	ALA	105	17.581	30.013	37.154	1.00	17.66
ATOM	452	C	ALA	105	16.348	28.433	35.710	1.00	2.00
ATOM	453	O	ALA	105	15.419	27.836	36.240	1.00	17.66
ATOM	454	N	LYS	106	16.307	28.827	34.444	1.00	11.55
ATOM	455	CA	LYS	106	15.109	28.606	33.635	1.00	11.55
ATOM	456	CB	LYS	106	15.102	29.507	32.392	1.00	26.36
ATOM	457	CG	LYS	106	14.999	31.015	32.716	1.00	26.36
ATOM	458	CD	LYS	106	14.630	31.862	31.518	1.00	26.36
ATOM	459	CE	LYS	106	13.149	31.713	31.135	1.00	26.36
ATOM	460	NZ	LYS	106	12.724	30.333	30.676	1.00	26.36
ATOM	461	C	LYS	106	14.982	27.132	33.251	1.00	11.55
ATOM	462	O	LYS	106	13.892	26.554	33.326	1.00	26.36
ATOM	463	N	ARG	107	16.109	26.516	32.898	1.00	16.17
ATOM	464	CA	ARG	107	16.131	25.111	32.524	1.00	16.17
ATOM	465	CB	ARG	107	17.491	24.743	31.938	1.00	38.14
ATOM	466	CG	ARG	107	17.492	23.395	31.262	1.00	38.14
ATOM	467	CD	ARG	107	18.669	23.246	30.326	1.00	38.14
ATOM	468	NE	ARG	107	18.425	22.252	29.275	1.00	38.14
ATOM	469	CZ	ARG	107	17.632	22.439	28.214	1.00	38.14
ATOM	470	NH1	ARG	107	16.979	23.593	28.034	1.00	38.14

FIG. 3I

ATOM	471	NH2	ARG	107	17.533	21.479	27.296	1.00	38.14
ATOM	472	C	ARG	107	15.790	24.179	33.697	1.00	16.17
ATOM	473	O	ARG	107	14.959	23.275	33.551	1.00	38.14
ATOM	474	N	ALA	108	16.441	24.396	34.844	1.00	17.90
ATOM	475	CA	ALA	108	16.218	23.606	36.058	1.00	17.90
ATOM	476	CB	ALA	108	17.224	23.987	37.114	1.00	2.00
ATOM	477	C	ALA	108	14.796	23.753	36.609	1.00	17.90
ATOM	478	O	ALA	108	14.223	22.790	37.115	1.00	2.00
ATOM	479	N	TYR	109	14.219	24.944	36.502	1.00	2.00
ATOM	480	CA	TYR	109	12.875	25.158	36.987	1.00	2.00
ATOM	481	CB	TYR	109	12.548	26.642	37.069	1.00	6.75
ATOM	482	CG	TYR	109	11.139	26.885	37.544	1.00	6.75
ATOM	483	CD1	TYR	109	10.791	26.671	38.871	1.00	6.75
ATOM	484	CE1	TYR	109	9.487	26.868	39.314	1.00	6.75
ATOM	485	CD2	TYR	109	10.146	27.308	36.668	1.00	6.75
ATOM	486	CE2	TYR	109	8.840	27.511	37.106	1.00	6.75
ATOM	487	CZ	TYR	109	8.518	27.290	38.430	1.00	6.75
ATOM	488	OH	TYR	109	7.235	27.513	38.878	1.00	6.75
ATOM	489	C	TYR	109	11.857	24.463	36.100	1.00	2.00
ATOM	490	O	TYR	109	10.923	23.840	36.589	1.00	6.75
ATOM	491	N	ARG	110	12.027	24.630	34.793	1.00	20.21
ATOM	492	CA	ARG	110	11.162	24.042	33.771	1.00	20.21
ATOM	493	CB	ARG	110	11.536	24.628	32.414	1.00	16.32
ATOM	494	CG	ARG	110	10.586	24.328	31.279	1.00	16.32
ATOM	495	CD	ARG	110	10.990	25.137	30.058	1.00	16.32
ATOM	496	NE	ARG	110	10.184	24.829	28.884	1.00	16.32
ATOM	497	CZ	ARG	110	10.648	24.190	27.817	1.00	16.32
ATOM	498	NH1	ARG	110	11.915	23.799	27.780	1.00	16.32
ATOM	499	NH2	ARG	110	9.846	23.940	26.788	1.00	16.32
ATOM	500	C	ARG	110	11.314	22.521	33.754	1.00	20.21
ATOM	501	O	ARG	110	10.361	21.793	33.482	1.00	16.32
ATOM	502	N	GLU	111	12.525	22.046	34.019	1.00	2.00
ATOM	503	CA	GLU	111	12.800	20.620	34.078	1.00	2.00
ATOM	504	CB	GLU	111	14.287	20.396	34.387	1.00	23.79
ATOM	505	CG	GLU	111	14.728	18.938	34.585	1.00	23.79
ATOM	506	CD	GLU	111	16.264	18.775	34.635	1.00	23.79
ATOM	507	OE1	GLU	111	16.753	17.651	34.352	1.00	23.79
ATOM	508	OE2	GLU	111	16.974	19.772	34.948	1.00	23.79
ATOM	509	C	GLU	111	11.932	20.029	35.189	1.00	2.00
ATOM	510	O	GLU	111	11.141	19.127	34.954	1.00	23.79
ATOM	511	N	LEU	112	12.045	20.599	36.384	1.00	21.88
ATOM	512	CA	LEU	112	11.288	20.171	37.559	1.00	21.88
ATOM	513	CB	LEU	112	11.518	21.150	38.701	1.00	6.65
ATOM	514	CG	LEU	112	12.563	20.834	39.746	1.00	6.65
ATOM	515	CD1	LEU	112	12.811	22.079	40.558	1.00	6.65
ATOM	516	CD2	LEU	112	12.065	19.700	40.605	1.00	6.65
ATOM	517	C	LEU	112	9.792	20.105	37.333	1.00	21.88
ATOM	518	O	LEU	112	9.156	19.092	37.609	1.00	6.65
ATOM	519	N	VAL	113	9.239	21.212	36.851	1.00	2.68
ATOM	520	CA	VAL	113	7.812	21.344	36.614	1.00	2.68
ATOM	521	CB	VAL	113	7.452	22.784	36.139	1.00	23.11
ATOM	522	CG1	VAL	113	5.945	22.958	36.101	1.00	23.11
ATOM	523	CG2	VAL	113	8.092	23.836	37.059	1.00	23.11
ATOM	524	C	VAL	113	7.239	20.321	35.639	1.00	2.68
ATOM	525	O	VAL	113	6.336	19.569	35.991	1.00	23.11
ATOM	526	N	LEU	114	7.800	20.251	34.437	1.00	19.44
ATOM	527	CA	LEU	114	7.321	19.327	33.413	1.00	19.44
ATOM	528	CB	LEU	114	7.894	19.701	32.054	1.00	5.29
ATOM	529	CG	LEU	114	7.360	21.018	31.517	1.00	5.29

FIG. 3J

ATOM	530	CD1	LEU	114	8.103	21.355	30.254	1.00	5.29
ATOM	531	CD2	LEU	114	5.862	20.915	31.278	1.00	5.29
ATOM	532	C	LEU	114	7.606	17.869	33.714	1.00	19.44
ATOM	533	O	LEU	114	6.760	17.000	33.488	1.00	5.29
ATOM	534	N	MET	115	8.793	17.590	34.227	1.00	2.00
ATOM	535	CA	MET	115	9.128	16.227	34.565	1.00	2.00
ATOM	536	CB	MET	115	10.598	16.115	34.949	1.00	7.04
ATOM	537	CG	MET	115	11.196	14.779	34.598	1.00	7.04
ATOM	538	SD	MET	115	12.885	14.586	35.145	1.00	7.04
ATOM	539	CE	MET	115	13.731	15.695	34.061	1.00	7.04
ATOM	540	C	MET	115	8.239	15.774	35.727	1.00	2.00
ATOM	541	O	MET	115	8.217	14.597	36.067	1.00	7.04
ATOM	542	N	LYS	116	7.515	16.716	36.335	1.00	7.50
ATOM	543	CA	LYS	116	6.624	16.408	37.443	1.00	7.50
ATOM	544	CB	LYS	116	6.748	17.443	38.561	1.00	25.41
ATOM	545	CG	LYS	116	7.889	17.235	39.557	1.00	25.41
ATOM	546	CD	LYS	116	7.633	18.102	40.780	1.00	25.41
ATOM	547	CE	LYS	116	8.655	17.895	41.893	1.00	25.41
ATOM	548	NZ	LYS	116	8.311	18.681	43.125	1.00	25.41
ATOM	549	C	LYS	116	5.161	16.296	37.044	1.00	7.50
ATOM	550	O	LYS	116	4.409	15.572	37.692	1.00	25.41
ATOM	551	N	CYS	117	4.764	16.993	35.978	1.00	18.55
ATOM	552	CA	CYS	117	3.368	16.987	35.509	1.00	18.55
ATOM	553	CB	CYS	117	2.865	18.421	35.322	1.00	28.53
ATOM	554	SG	CYS	117	3.668	19.290	33.963	1.00	28.53
ATOM	555	C	CYS	117	3.083	16.188	34.225	1.00	18.55
ATOM	556	O	CYS	117	1.919	15.914	33.908	1.00	28.53
ATOM	557	N	VAL	118	4.135	15.847	33.482	1.00	13.50
ATOM	558	CA	VAL	118	4.005	15.086	32.242	1.00	13.50
ATOM	559	CB	VAL	118	5.103	15.475	31.230	1.00	25.80
ATOM	560	CG1	VAL	118	4.988	14.640	29.972	1.00	25.80
ATOM	561	CG2	VAL	118	5.014	16.942	30.906	1.00	25.80
ATOM	562	C	VAL	118	4.163	13.604	32.528	1.00	13.50
ATOM	563	O	VAL	118	5.118	13.199	33.201	1.00	25.80
ATOM	564	N	THR	119	3.244	12.784	32.021	1.00	29.88
ATOM	565	CA	THR	119	3.346	11.344	32.239	1.00	29.88
ATOM	566	CB	THR	119	2.433	10.845	33.386	1.00	46.17
ATOM	567	OG1	THR	119	2.862	9.540	33.795	1.00	46.17
ATOM	568	CG2	THR	119	0.954	10.796	32.961	1.00	46.17
ATOM	569	C	THR	119	3.153	10.534	30.966	1.00	29.88
ATOM	570	O	THR	119	2.049	10.406	30.424	1.00	46.17
ATOM	571	N	HIS	120	4.264	9.982	30.498	1.00	11.14
ATOM	572	CA	HIS	120	4.270	9.200	29.278	1.00	11.14
ATOM	573	CB	HIS	120	4.422	10.139	28.094	1.00	12.95
ATOM	574	CG	HIS	120	4.469	9.443	26.767	1.00	12.95
ATOM	575	CD2	HIS	120	5.426	9.387	25.825	1.00	12.95
ATOM	576	ND1	HIS	120	3.416	8.680	26.302	1.00	12.95
ATOM	577	CE1	HIS	120	3.737	8.183	25.118	1.00	12.95
ATOM	578	NE2	HIS	120	4.947	8.594	24.805	1.00	12.95
ATOM	579	C	HIS	120	5.432	8.227	29.351	1.00	11.14
ATOM	580	O	HIS	120	6.454	8.526	29.966	1.00	12.95
ATOM	581	N	LYS	121	5.271	7.071	28.717	1.00	2.00
ATOM	582	CA	LYS	121	6.294	6.036	28.730	1.00	2.00
ATOM	583	CB	LYS	121	5.700	4.697	28.281	1.00	11.42
ATOM	584	CG	LYS	121	5.028	4.721	26.918	1.00	11.42
ATOM	585	CD	LYS	121	4.423	3.362	26.545	1.00	11.42
ATOM	586	CE	LYS	121	5.478	2.269	26.451	1.00	11.42
ATOM	587	NZ	LYS	121	6.495	2.546	25.396	1.00	11.42
ATOM	588	C	LYS	121	7.550	6.349	27.928	1.00	2.00

FIG. 3K

ATOM	589	O	LYS	121	8.584	5.713	28.124	1.00	11.42
ATOM	590	N	ASN	122	7.475	7.370	27.073	1.00	13.02
ATOM	591	CA	ASN	122	8.605	7.763	26.220	1.00	13.02
ATOM	592	CB	ASN	122	8.180	7.770	24.753	1.00	2.00
ATOM	593	CG	ASN	122	7.642	6.432	24.295	1.00	2.00
ATOM	594	OD1	ASN	122	6.520	6.337	23.812	1.00	2.00
ATOM	595	ND2	ASN	122	8.438	5.385	24.470	1.00	2.00
ATOM	596	C	ASN	122	9.242	9.089	26.592	1.00	13.02
ATOM	597	O	ASN	122	10.095	9.596	25.863	1.00	2.00
ATOM	598	N	ILE	123	8.788	9.647	27.715	1.00	11.02
ATOM	599	CA	ILE	123	9.282	10.903	28.283	1.00	11.02
ATOM	600	CB	ILE	123	8.175	11.965	28.434	1.00	2.63
ATOM	601	CG2	ILE	123	8.750	13.204	29.091	1.00	2.63
ATOM	602	CG1	ILE	123	7.588	12.333	27.074	1.00	2.63
ATOM	603	CD1	ILE	123	8.553	13.063	26.168	1.00	2.63
ATOM	604	C	ILE	123	9.759	10.514	29.671	1.00	11.02
ATOM	605	O	ILE	123	9.046	9.825	30.397	1.00	2.63
ATOM	606	N	ILE	124	10.932	10.998	30.070	1.00	18.75
ATOM	607	CA	ILE	124	11.501	10.629	31.368	1.00	18.75
ATOM	608	CB	ILE	124	12.940	11.205	31.577	1.00	5.83
ATOM	609	CG2	ILE	124	12.891	12.679	31.928	1.00	5.83
ATOM	610	CG1	ILE	124	13.693	10.418	32.650	1.00	5.83
ATOM	611	CD1	ILE	124	14.175	9.055	32.209	1.00	5.83
ATOM	612	C	ILE	124	10.602	10.926	32.569	1.00	18.75
ATOM	613	O	ILE	124	9.856	11.916	32.604	1.00	5.83
ATOM	614	N	SER	125	10.626	9.978	33.505	1.00	32.81
ATOM	615	CA	SER	125	9.846	10.012	34.740	1.00	32.81
ATOM	616	CB	SER	125	9.218	8.631	34.983	1.00	33.06
ATOM	617	OG	SER	125	10.203	7.594	35.025	1.00	33.06
ATOM	618	C	SER	125	10.698	10.393	35.937	1.00	32.81
ATOM	619	O	SER	125	11.807	9.881	36.126	1.00	33.06
ATOM	620	N	LEU	126	10.163	11.299	36.742	1.00	19.68
ATOM	621	CA	LEU	126	10.849	11.761	37.937	1.00	19.68
ATOM	622	CB	LEU	126	10.559	13.246	38.161	1.00	2.00
ATOM	623	CG	LEU	126	11.407	13.970	39.195	1.00	2.00
ATOM	624	CD1	LEU	126	12.855	13.566	39.085	1.00	2.00
ATOM	625	CD2	LEU	126	11.254	15.460	38.982	1.00	2.00
ATOM	626	C	LEU	126	10.387	10.919	39.127	1.00	19.68
ATOM	627	O	LEU	126	9.218	10.937	39.503	1.00	2.00
ATOM	628	N	LEU	127	11.311	10.129	39.659	1.00	23.39
ATOM	629	CA	LEU	127	11.040	9.251	40.794	1.00	23.39
ATOM	630	CB	LEU	127	11.991	8.051	40.765	1.00	2.00
ATOM	631	CG	LEU	127	11.746	6.927	39.773	1.00	2.00
ATOM	632	CD1	LEU	127	12.846	5.917	39.958	1.00	2.00
ATOM	633	CD2	LEU	127	10.390	6.305	40.018	1.00	2.00
ATOM	634	C	LEU	127	11.111	9.910	42.182	1.00	23.39
ATOM	635	O	LEU	127	10.273	9.631	43.044	1.00	2.00
ATOM	636	N	ASN	128	12.098	10.779	42.387	1.00	2.00
ATOM	637	CA	ASN	128	12.267	11.440	43.668	1.00	2.00
ATOM	638	CB	ASN	128	12.896	10.460	44.659	1.00	16.49
ATOM	639	CG	ASN	128	12.913	10.979	46.077	1.00	16.49
ATOM	640	OD1	ASN	128	12.031	11.729	46.494	1.00	16.49
ATOM	641	ND2	ASN	128	13.903	10.556	46.839	1.00	16.49
ATOM	642	C	ASN	128	13.128	12.685	43.542	1.00	2.00
ATOM	643	O	ASN	128	14.205	12.649	42.957	1.00	16.49
ATOM	644	N	VAL	129	12.649	13.786	44.106	1.00	19.28
ATOM	645	CA	VAL	129	13.376	15.050	44.072	1.00	19.28
ATOM	646	CB	VAL	129	12.480	16.199	43.553	1.00	10.22
ATOM	647	CG1	VAL	129	13.340	17.360	43.058	1.00	10.22

FIG. 3L

ATOM	648	CG2	VAL	129	11.543	15.699	42.478	1.00	10.22
ATOM	649	C	VAL	129	13.769	15.374	45.504	1.00	19.28
ATOM	650	O	VAL	129	12.944	15.238	46.401	1.00	10.22
ATOM	651	N	PHE	130	15.020	15.765	45.733	1.00	13.60
ATOM	652	CA	PHE	130	15.440	16.107	47.084	1.00	13.60
ATOM	653	CB	PHE	130	15.681	14.838	47.923	1.00	3.04
ATOM	654	CG	PHE	130	16.870	14.036	47.487	1.00	3.04
ATOM	655	CD1	PHE	130	18.136	14.317	47.987	1.00	3.04
ATOM	656	CD2	PHE	130	16.721	13.012	46.566	1.00	3.04
ATOM	657	CE1	PHE	130	19.238	13.595	47.575	1.00	3.04
ATOM	658	CE2	PHE	130	17.810	12.279	46.140	1.00	3.04
ATOM	659	CZ	PHE	130	19.078	12.572	46.645	1.00	3.04
ATOM	660	C	PHE	130	16.637	17.038	47.182	1.00	13.60
ATOM	661	O	PHE	130	17.422	17.179	46.244	1.00	3.04
ATOM	662	N	THR	131	16.746	17.677	48.345	1.00	2.00
ATOM	663	CA	THR	131	17.831	18.588	48.643	1.00	2.00
ATOM	664	CB	THR	131	17.365	20.080	48.645	1.00	12.19
ATOM	665	OG1	THR	131	18.444	20.930	49.036	1.00	12.19
ATOM	666	CG2	THR	131	16.190	20.301	49.583	1.00	12.19
ATOM	667	C	THR	131	18.424	18.243	50.001	1.00	2.00
ATOM	668	O	THR	131	17.706	17.952	50.957	1.00	12.19
ATOM	669	N	PRO	132	19.753	18.182	50.072	1.00	3.54
ATOM	670	CD	PRO	132	20.704	18.219	48.952	1.00	3.20
ATOM	671	CA	PRO	132	20.447	17.875	51.315	1.00	3.54
ATOM	672	CB	PRO	132	21.815	17.428	50.827	1.00	3.20
ATOM	673	CG	PRO	132	22.045	18.285	49.661	1.00	3.20
ATOM	674	C	PRO	132	20.545	19.130	52.189	1.00	3.54
ATOM	675	O	PRO	132	21.321	19.164	53.141	1.00	3.20
ATOM	676	N	GLN	133	19.817	20.183	51.825	1.00	4.78
ATOM	677	CA	GLN	133	19.837	21.417	52.594	1.00	4.78
ATOM	678	CB	GLN	133	20.255	22.593	51.726	1.00	4.25
ATOM	679	CG	GLN	133	21.706	22.500	51.244	1.00	4.25
ATOM	680	CD	GLN	133	21.842	22.103	49.776	1.00	4.25
ATOM	681	OE1	GLN	133	22.938	21.782	49.313	1.00	4.25
ATOM	682	NE2	GLN	133	20.740	22.158	49.031	1.00	4.25
ATOM	683	C	GLN	133	18.491	21.664	53.261	1.00	4.78
ATOM	684	O	GLN	133	17.438	21.627	52.614	1.00	4.25
ATOM	685	N	LYS	134	18.543	21.913	54.570	1.00	33.73
ATOM	686	CA	LYS	134	17.347	22.134	55.373	1.00	33.73
ATOM	687	CB	LYS	134	17.641	21.862	56.857	1.00	32.87
ATOM	688	CG	LYS	134	17.725	20.379	57.225	1.00	32.87
ATOM	689	CD	LYS	134	16.352	19.667	57.154	1.00	32.87
ATOM	690	CE	LYS	134	16.477	18.156	57.418	1.00	32.87
ATOM	691	NZ	LYS	134	17.282	17.463	56.353	1.00	32.87
ATOM	692	C	LYS	134	16.658	23.482	55.220	1.00	33.73
ATOM	693	O	LYS	134	15.423	23.541	55.152	1.00	32.87
ATOM	694	N	THR	135	17.445	24.558	55.169	1.00	47.73
ATOM	695	CA	THR	135	16.883	25.905	55.046	1.00	47.73
ATOM	696	CB	THR	135	17.509	26.874	56.046	1.00	14.84
ATOM	697	OG1	THR	135	18.863	27.134	55.663	1.00	14.84
ATOM	698	CG2	THR	135	17.472	26.278	57.447	1.00	14.84
ATOM	699	C	THR	135	16.987	26.548	53.673	1.00	47.73
ATOM	700	O	THR	135	17.947	26.333	52.935	1.00	14.84
ATOM	701	N	LEU	136	16.040	27.442	53.412	1.00	2.00
ATOM	702	CA	LEU	136	15.947	28.175	52.161	1.00	2.00
ATOM	703	CB	LEU	136	14.675	29.013	52.200	1.00	7.33
ATOM	704	CG	LEU	136	14.233	29.957	51.082	1.00	7.33
ATOM	705	CD1	LEU	136	14.722	29.512	49.713	1.00	7.33
ATOM	706	CD2	LEU	136	12.702	30.046	51.146	1.00	7.33

FIG. 3M

ATOM	707	C	LEU	136	17.183	29.042	51.963	1.00	2.00
ATOM	708	O	LEU	136	17.423	29.556	50.879	1.00	7.33
ATOM	709	N	GLU	137	17.952	29.217	53.034	1.00	31.36
ATOM	710	CA	GLU	137	19.174	29.997	52.971	1.00	31.36
ATOM	711	CB	GLU	137	19.468	30.699	54.311	1.00	31.26
ATOM	712	CG	GLU	137	18.689	31.988	54.571	1.00	31.26
ATOM	713	CD	GLU	137	17.217	31.746	54.824	1.00	31.26
ATOM	714	OE1	GLU	137	16.874	31.316	55.954	1.00	31.26
ATOM	715	OE2	GLU	137	16.408	31.995	53.897	1.00	31.26
ATOM	716	C	GLU	137	20.308	29.046	52.643	1.00	31.36
ATOM	717	O	GLU	137	21.187	29.365	51.843	1.00	31.26
ATOM	718	N	GLU	138	20.296	27.885	53.290	1.00	18.21
ATOM	719	CA	GLU	138	21.323	26.876	53.059	1.00	18.21
ATOM	720	CB	GLU	138	21.201	25.760	54.080	1.00	15.04
ATOM	721	CG	GLU	138	21.529	26.161	55.492	1.00	15.04
ATOM	722	CD	GLU	138	21.167	25.065	56.475	1.00	15.04
ATOM	723	OE1	GLU	138	20.996	25.388	57.667	1.00	15.04
ATOM	724	OE2	GLU	138	21.046	23.881	56.049	1.00	15.04
ATOM	725	C	GLU	138	21.215	26.264	51.668	1.00	18.21
ATOM	726	O	GLU	138	22.184	25.693	51.167	1.00	15.04
ATOM	727	N	PHE	139	20.026	26.381	51.078	1.00	16.05
ATOM	728	CA	PHE	139	19.706	25.843	49.766	1.00	16.05
ATOM	729	CB	PHE	139	18.343	26.391	49.310	1.00	31.29
ATOM	730	CG	PHE	139	17.847	25.800	48.009	1.00	31.29
ATOM	731	CD1	PHE	139	17.879	24.422	47.802	1.00	31.29
ATOM	732	CD2	PHE	139	17.385	26.619	46.982	1.00	31.29
ATOM	733	CE1	PHE	139	17.467	23.867	46.588	1.00	31.29
ATOM	734	CE2	PHE	139	16.967	26.082	45.760	1.00	31.29
ATOM	735	CZ	PHE	139	17.008	24.703	45.561	1.00	31.29
ATOM	736	C	PHE	139	20.786	26.105	48.709	1.00	16.05
ATOM	737	O	PHE	139	21.061	27.256	48.350	1.00	31.29
ATOM	738	N	GLN	140	21.414	25.036	48.231	1.00	2.00
ATOM	739	CA	GLN	140	22.466	25.157	47.241	1.00	2.00
ATOM	740	CB	GLN	140	23.820	24.911	47.898	1.00	31.26
ATOM	741	CG	GLN	140	24.966	25.054	46.954	1.00	31.26
ATOM	742	CD	GLN	140	26.264	25.266	47.672	1.00	31.26
ATOM	743	OE1	GLN	140	26.386	26.183	48.482	1.00	31.26
ATOM	744	NE2	GLN	140	27.253	24.416	47.386	1.00	31.26
ATOM	745	C	GLN	140	22.287	24.258	46.020	1.00	2.00
ATOM	746	O	GLN	140	22.262	24.757	44.894	1.00	31.26
ATOM	747	N	ASP	141	22.185	22.946	46.230	1.00	10.22
ATOM	748	CA	ASP	141	22.022	22.008	45.125	1.00	10.22
ATOM	749	CB	ASP	141	23.152	20.980	45.123	1.00	13.10
ATOM	750	CG	ASP	141	24.524	21.613	45.146	1.00	13.10
ATOM	751	OD1	ASP	141	24.732	22.666	44.515	1.00	13.10
ATOM	752	OD2	ASP	141	25.418	21.070	45.815	1.00	13.10
ATOM	753	C	ASP	141	20.684	21.285	45.179	1.00	10.22
ATOM	754	O	ASP	141	19.991	21.323	46.199	1.00	13.10
ATOM	755	N	VAL	142	20.308	20.675	44.055	1.00	6.00
ATOM	756	CA	VAL	142	19.070	19.901	43.923	1.00	6.00
ATOM	757	CB	VAL	142	18.043	20.631	43.043	1.00	2.00
ATOM	758	CG1	VAL	142	16.789	19.783	42.866	1.00	2.00
ATOM	759	CG2	VAL	142	17.696	21.962	43.672	1.00	2.00
ATOM	760	C	VAL	142	19.425	18.552	43.296	1.00	6.00
ATOM	761	O	VAL	142	20.270	18.486	42.412	1.00	2.00
ATOM	762	N	TYR	143	18.814	17.475	43.789	1.00	3.45
ATOM	763	CA	TYR	143	19.089	16.130	43.289	1.00	3.45
ATOM	764	CB	TYR	143	19.607	15.227	44.405	1.00	2.80
ATOM	765	CG	TYR	143	20.990	15.557	44.878	1.00	2.80

FIG. 3N

ATOM	766	CD1	TYR	143	21.217	16.619	45.739	1.00	2.80
ATOM	767	CE1	TYR	143	22.493	16.932	46.171	1.00	2.80
ATOM	768	CD2	TYR	143	22.078	14.813	44.459	1.00	2.80
ATOM	769	CE2	TYR	143	23.362	15.120	44.882	1.00	2.80
ATOM	770	CZ	TYR	143	23.567	16.184	45.736	1.00	2.80
ATOM	771	OH	TYR	143	24.849	16.513	46.129	1.00	2.80
ATOM	772	C	TYR	143	17.848	15.509	42.691	1.00	3.45
ATOM	773	O	TYR	143	16.846	15.331	43.376	1.00	2.80
ATOM	774	N	LEU	144	17.915	15.193	41.401	1.00	20.45
ATOM	775	CA	LEU	144	16.789	14.578	40.694	1.00	20.45
ATOM	776	CB	LEU	144	16.635	15.173	39.284	1.00	5.98
ATOM	777	CG	LEU	144	16.571	16.690	39.101	1.00	5.98
ATOM	778	CD1	LEU	144	16.787	17.000	37.651	1.00	5.98
ATOM	779	CD2	LEU	144	15.246	17.268	39.574	1.00	5.98
ATOM	780	C	LEU	144	17.032	13.078	40.575	1.00	20.45
ATOM	781	O	LEU	144	18.152	12.639	40.286	1.00	5.98
ATOM	782	N	VAL	145	15.991	12.294	40.835	1.00	6.79
ATOM	783	CA	VAL	145	16.102	10.841	40.738	1.00	6.79
ATOM	784	CB	VAL	145	15.889	10.161	42.113	1.00	2.00
ATOM	785	CG1	VAL	145	15.824	8.671	41.951	1.00	2.00
ATOM	786	CG2	VAL	145	17.015	10.525	43.056	1.00	2.00
ATOM	787	C	VAL	145	15.124	10.269	39.720	1.00	6.79
ATOM	788	O	VAL	145	13.911	10.416	39.853	1.00	2.00
ATOM	789	N	MET	146	15.652	9.658	38.671	1.00	19.74
ATOM	790	CA	MET	146	14.792	9.060	37.657	1.00	19.74
ATOM	791	CB	MET	146	14.943	9.773	36.319	1.00	10.11
ATOM	792	CG	MET	146	14.723	11.253	36.405	1.00	10.11
ATOM	793	SD	MET	146	16.115	12.116	35.673	1.00	10.11
ATOM	794	CE	MET	146	17.511	11.529	36.681	1.00	10.11
ATOM	795	C	MET	146	15.189	7.607	37.533	1.00	19.74
ATOM	796	O	MET	146	15.972	7.101	38.329	1.00	10.11
ATOM	797	N	GLU	147	14.654	6.934	36.526	1.00	2.00
ATOM	798	CA	GLU	147	14.961	5.531	36.312	1.00	2.00
ATOM	799	CB	GLU	147	13.923	4.906	35.419	1.00	35.81
ATOM	800	CG	GLU	147	12.537	5.132	35.881	1.00	35.81
ATOM	801	CD	GLU	147	11.530	4.438	35.011	1.00	35.81
ATOM	802	OE1	GLU	147	11.914	3.602	34.152	1.00	35.81
ATOM	803	OE2	GLU	147	10.338	4.732	35.201	1.00	35.81
ATOM	804	C	GLU	147	16.299	5.352	35.658	1.00	2.00
ATOM	805	O	GLU	147	16.846	6.274	35.067	1.00	35.81
ATOM	806	N	LEU	148	16.801	4.135	35.720	1.00	2.00
ATOM	807	CA	LEU	148	18.060	3.847	35.097	1.00	2.00
ATOM	808	CB	LEU	148	18.962	3.091	36.052	1.00	2.00
ATOM	809	CG	LEU	148	20.399	3.148	35.568	1.00	2.00
ATOM	810	CD1	LEU	148	20.940	4.544	35.769	1.00	2.00
ATOM	811	CD2	LEU	148	21.228	2.139	36.303	1.00	2.00
ATOM	812	C	LEU	148	17.872	3.066	33.792	1.00	2.00
ATOM	813	O	LEU	148	17.317	1.963	33.759	1.00	2.00
ATOM	814	N	MET	149	18.305	3.698	32.711	1.00	12.82
ATOM	815	CA	MET	149	18.251	3.120	31.387	1.00	12.82
ATOM	816	CB	MET	149	18.097	4.207	30.335	1.00	5.88
ATOM	817	CG	MET	149	16.934	5.107	30.610	1.00	5.88
ATOM	818	SD	MET	149	15.478	4.137	30.863	1.00	5.88
ATOM	819	CE	MET	149	14.727	4.271	29.246	1.00	5.88
ATOM	820	C	MET	149	19.585	2.434	31.218	1.00	12.82
ATOM	821	O	MET	149	20.474	2.572	32.065	1.00	5.88
ATOM	822	N	ASP	150	19.741	1.723	30.106	1.00	5.65
ATOM	823	CA	ASP	150	20.971	0.996	29.856	1.00	5.65
ATOM	824	CB	ASP	150	20.631	-0.351	29.256	1.00	4.35

FIG. 30

ATOM	825	CG	ASP	150	19.680	-1.122	30.110	1.00	4.35
ATOM	826	OD1	ASP	150	19.847	-1.096	31.342	1.00	4.35
ATOM	827	OD2	ASP	150	18.746	-1.729	29.575	1.00	4.35
ATOM	828	C	ASP	150	22.042	1.695	29.067	1.00	5.65
ATOM	829	O	ASP	150	23.211	1.326	29.168	1.00	4.35
ATOM	830	N	ALA	151	21.654	2.701	28.292	1.00	2.00
ATOM	831	CA	ALA	151	22.595	3.461	27.474	1.00	2.00
ATOM	832	CB	ALA	151	23.152	2.568	26.364	1.00	2.00
ATOM	833	C	ALA	151	21.920	4.673	26.855	1.00	2.00
ATOM	834	O	ALA	151	20.741	4.914	27.071	1.00	2.00
ATOM	835	N	ASN	152	22.692	5.445	26.100	1.00	23.78
ATOM	836	CA	ASN	152	22.163	6.613	25.401	1.00	23.78
ATOM	837	CB	ASN	152	23.103	7.832	25.525	1.00	36.42
ATOM	838	CG	ASN	152	24.481	7.596	24.918	1.00	36.42
ATOM	839	OD1	ASN	152	24.621	6.905	23.910	1.00	36.42
ATOM	840	ND2	ASN	152	25.499	8.190	25.524	1.00	36.42
ATOM	841	C	ASN	152	21.906	6.262	23.921	1.00	23.78
ATOM	842	O	ASN	152	22.289	5.186	23.446	1.00	36.42
ATOM	843	N	LEU	153	21.282	7.182	23.193	1.00	11.01
ATOM	844	CA	LEU	153	20.984	6.954	21.783	1.00	11.01
ATOM	845	CB	LEU	153	19.923	7.924	21.297	1.00	2.00
ATOM	846	CG	LEU	153	18.761	7.314	20.526	1.00	2.00
ATOM	847	CD1	LEU	153	18.173	8.369	19.610	1.00	2.00
ATOM	848	CD2	LEU	153	19.220	6.129	19.727	1.00	2.00
ATOM	849	C	LEU	153	22.208	7.056	20.872	1.00	11.01
ATOM	850	O	LEU	153	22.203	6.504	19.783	1.00	2.00
ATOM	851	N	CYS	154	23.260	7.728	21.330	1.00	12.15
ATOM	852	CA	CYS	154	24.462	7.890	20.532	1.00	12.15
ATOM	853	CB	CYS	154	25.243	9.131	20.964	1.00	53.10
ATOM	854	SG	CYS	154	26.248	8.917	22.444	1.00	53.10
ATOM	855	C	CYS	154	25.337	6.645	20.589	1.00	12.15
ATOM	856	O	CYS	154	26.325	6.538	19.862	1.00	53.10
ATOM	857	N	GLN	155	24.971	5.713	21.466	1.00	2.99
ATOM	858	CA	GLN	155	25.683	4.455	21.604	1.00	2.99
ATOM	859	CB	GLN	155	25.533	3.913	23.016	1.00	16.88
ATOM	860	CG	GLN	155	26.518	4.461	24.027	1.00	16.88
ATOM	861	CD	GLN	155	26.286	3.868	25.414	1.00	16.88
ATOM	862	OE1	GLN	155	25.385	4.292	26.139	1.00	16.88
ATOM	863	NE2	GLN	155	27.088	2.872	25.777	1.00	16.88
ATOM	864	C	GLN	155	25.033	3.488	20.635	1.00	2.99
ATOM	865	O	GLN	155	25.693	2.638	20.055	1.00	16.88
ATOM	866	N	VAL	156	23.721	3.637	20.484	1.00	12.86
ATOM	867	CA	VAL	156	22.916	2.816	19.579	1.00	12.86
ATOM	868	CB	VAL	156	21.399	3.055	19.839	1.00	2.00
ATOM	869	CG1	VAL	156	20.539	2.462	18.731	1.00	2.00
ATOM	870	CG2	VAL	156	20.999	2.484	21.181	1.00	2.00
ATOM	871	C	VAL	156	23.249	3.203	18.123	1.00	12.86
ATOM	872	O	VAL	156	22.997	2.460	17.175	1.00	2.00
ATOM	873	N	ILE	157	23.834	4.380	17.970	1.00	10.11
ATOM	874	CA	ILE	157	24.213	4.893	16.683	1.00	10.11
ATOM	875	CB	ILE	157	24.291	6.432	16.755	1.00	8.01
ATOM	876	CG2	ILE	157	25.350	6.997	15.812	1.00	8.01
ATOM	877	CG1	ILE	157	22.904	6.994	16.453	1.00	8.01
ATOM	878	CD1	ILE	157	22.730	8.386	16.893	1.00	8.01
ATOM	879	C	ILE	157	25.520	4.263	16.235	1.00	10.11
ATOM	880	O	ILE	157	25.806	4.196	15.039	1.00	8.01
ATOM	881	N	GLN	158	26.286	3.743	17.184	1.00	2.00
ATOM	882	CA	GLN	158	27.551	3.106	16.853	1.00	2.00
ATOM	883	CB	GLN	158	28.533	3.251	18.005	1.00	52.31

FIG. 3P

ATOM	884	CG	GLN	158	29.150	4.613	18.169	1.00	52.31
ATOM	885	CD	GLN	158	30.188	4.613	19.276	1.00	52.31
ATOM	886	OE1	GLN	158	31.112	3.786	19.272	1.00	52.31
ATOM	887	NE2	GLN	158	30.034	5.521	20.246	1.00	52.31
ATOM	888	C	GLN	158	27.396	1.628	16.507	1.00	2.00
ATOM	889	O	GLN	158	28.381	0.886	16.483	1.00	52.31
ATOM	890	N	MET	159	26.159	1.190	16.298	1.00	2.84
ATOM	891	CA	MET	159	25.890	-0.197	15.956	1.00	2.84
ATOM	892	CB	MET	159	25.516	-0.978	17.203	1.00	12.08
ATOM	893	CG	MET	159	24.130	-0.673	17.736	1.00	12.08
ATOM	894	SD	MET	159	24.057	-0.915	19.488	1.00	12.08
ATOM	895	CE	MET	159	22.779	-2.121	19.575	1.00	12.08
ATOM	896	C	MET	159	24.760	-0.265	14.937	1.00	2.84
ATOM	897	O	MET	159	23.749	0.428	15.059	1.00	12.08
ATOM	898	N	GLU	160	24.921	-1.118	13.937	1.00	2.00
ATOM	899	CA	GLU	160	23.916	-1.254	12.899	1.00	2.00
ATOM	900	CB	GLU	160	24.518	-1.933	11.663	1.00	23.86
ATOM	901	CG	GLU	160	25.306	-3.189	11.973	1.00	23.86
ATOM	902	CD	GLU	160	25.643	-3.988	10.730	1.00	23.86
ATOM	903	OE1	GLU	160	26.618	-3.623	10.031	1.00	23.86
ATOM	904	OE2	GLU	160	24.938	-4.987	10.471	1.00	23.86
ATOM	905	C	GLU	160	22.711	-2.032	13.396	1.00	2.00
ATOM	906	O	GLU	160	22.847	-3.137	13.899	1.00	23.86
ATOM	907	N	LEU	161	21.530	-1.443	13.254	1.00	5.79
ATOM	908	CA	LEU	161	20.292	-2.074	13.713	1.00	5.79
ATOM	909	CB	LEU	161	19.462	-1.071	14.510	1.00	13.20
ATOM	910	CG	LEU	161	20.034	-0.330	15.703	1.00	13.20
ATOM	911	CD1	LEU	161	19.066	0.772	16.064	1.00	13.20
ATOM	912	CD2	LEU	161	20.249	-1.293	16.857	1.00	13.20
ATOM	913	C	LEU	161	19.392	-2.600	12.598	1.00	5.79
ATOM	914	O	LEU	161	19.435	-2.113	11.466	1.00	13.20
ATOM	915	N	ASP	162	18.559	-3.582	12.933	1.00	7.84
ATOM	916	CA	ASP	162	17.606	-4.121	11.977	1.00	7.84
ATOM	917	CB	ASP	162	17.054	-5.477	12.449	1.00	9.47
ATOM	918	CG	ASP	162	16.717	-5.502	13.942	1.00	9.47
ATOM	919	OD1	ASP	162	17.654	-5.665	14.759	1.00	9.47
ATOM	920	OD2	ASP	162	15.517	-5.390	14.292	1.00	9.47
ATOM	921	C	ASP	162	16.478	-3.083	11.857	1.00	7.84
ATOM	922	O	ASP	162	16.405	-2.161	12.667	1.00	9.47
ATOM	923	N	HIS	163	15.629	-3.202	10.836	1.00	22.67
ATOM	924	CA	HIS	163	14.513	-2.265	10.642	1.00	22.67
ATOM	925	CB	HIS	163	13.807	-2.537	9.322	1.00	13.35
ATOM	926	CG	HIS	163	14.651	-2.254	8.127	1.00	13.35
ATOM	927	CD2	HIS	163	14.985	-3.032	7.069	1.00	13.35
ATOM	928	ND1	HIS	163	15.260	-1.038	7.916	1.00	13.35
ATOM	929	CE1	HIS	163	15.932	-1.074	6.783	1.00	13.35
ATOM	930	NE2	HIS	163	15.783	-2.275	6.249	1.00	13.35
ATOM	931	C	HIS	163	13.471	-2.255	11.764	1.00	22.67
ATOM	932	O	HIS	163	12.824	-1.238	11.987	1.00	13.35
ATOM	933	N	GLU	164	13.316	-3.379	12.465	1.00	21.78
ATOM	934	CA	GLU	164	12.345	-3.498	13.564	1.00	21.78
ATOM	935	CB	GLU	164	12.221	-4.960	14.005	1.00	11.17
ATOM	936	CG	GLU	164	11.194	-5.786	13.232	1.00	11.17
ATOM	937	CD	GLU	164	11.437	-5.819	11.734	1.00	11.17
ATOM	938	OE1	GLU	164	10.452	-5.639	10.989	1.00	11.17
ATOM	939	OE2	GLU	164	12.595	-6.035	11.294	1.00	11.17
ATOM	940	C	GLU	164	12.721	-2.631	14.760	1.00	21.78
ATOM	941	O	GLU	164	11.955	-1.782	15.206	1.00	11.17
ATOM	942	N	ARG	165	13.926	-2.845	15.257	1.00	2.00

FIG. 3Q

ATOM	943	CA	ARG	165	14.439	-2.094	16.373	1.00	2.00
ATOM	944	CB	ARG	165	15.839	-2.582	16.714	1.00	23.45
ATOM	945	CG	ARG	165	15.866	-3.907	17.467	1.00	23.45
ATOM	946	CD	ARG	165	17.304	-4.246	17.862	1.00	23.45
ATOM	947	NE	ARG	165	17.397	-5.350	18.807	1.00	23.45
ATOM	948	CZ	ARG	165	17.137	-6.622	18.516	1.00	23.45
ATOM	949	NH1	ARG	165	16.759	-6.984	17.297	1.00	23.45
ATOM	950	NH2	ARG	165	17.260	-7.542	19.454	1.00	23.45
ATOM	951	C	ARG	165	14.480	-0.624	16.017	1.00	2.00
ATOM	952	O	ARG	165	13.924	0.201	16.728	1.00	23.45
ATOM	953	N	MET	166	15.120	-0.310	14.897	1.00	2.00
ATOM	954	CA	MET	166	15.252	1.061	14.407	1.00	2.00
ATOM	955	CB	MET	166	15.915	1.046	13.031	1.00	28.00
ATOM	956	CG	MET	166	16.291	2.401	12.473	1.00	28.00
ATOM	957	SD	MET	166	16.936	2.244	10.786	1.00	28.00
ATOM	958	CE	MET	166	18.697	1.770	11.111	1.00	28.00
ATOM	959	C	MET	166	13.897	1.781	14.340	1.00	2.00
ATOM	960	O	MET	166	13.766	2.913	14.809	1.00	28.00
ATOM	961	N	SER	167	12.887	1.106	13.790	1.00	12.38
ATOM	962	CA	SER	167	11.537	1.655	13.666	1.00	12.38
ATOM	963	CB	SER	167	10.715	0.830	12.683	1.00	11.87
ATOM	964	OG	SER	167	10.651	-0.522	13.100	1.00	11.87
ATOM	965	C	SER	167	10.788	1.746	14.996	1.00	12.38
ATOM	966	O	SER	167	9.874	2.568	15.129	1.00	11.87
ATOM	967	N	TYR	168	11.130	0.891	15.962	1.00	2.00
ATOM	968	CA	TYR	168	10.481	0.938	17.266	1.00	2.00
ATOM	969	CB	TYR	168	10.763	-0.322	18.088	1.00	4.15
ATOM	970	CG	TYR	168	9.916	-0.389	19.328	1.00	4.15
ATOM	971	CD1	TYR	168	8.543	-0.155	19.263	1.00	4.15
ATOM	972	CE1	TYR	168	7.750	-0.148	20.406	1.00	4.15
ATOM	973	CD2	TYR	168	10.479	-0.629	20.571	1.00	4.15
ATOM	974	CE2	TYR	168	9.692	-0.625	21.733	1.00	4.15
ATOM	975	CZ	TYR	168	8.325	-0.381	21.642	1.00	4.15
ATOM	976	OH	TYR	168	7.544	-0.357	22.780	1.00	4.15
ATOM	977	C	TYR	168	11.007	2.162	18.004	1.00	2.00
ATOM	978	O	TYR	168	10.250	2.911	18.626	1.00	4.15
ATOM	979	N	LEU	169	12.317	2.352	17.919	1.00	4.07
ATOM	980	CA	LEU	169	12.970	3.482	18.526	1.00	4.07
ATOM	981	CB	LEU	169	14.482	3.400	18.292	1.00	4.89
ATOM	982	CG	LEU	169	15.256	2.291	19.009	1.00	4.89
ATOM	983	CD1	LEU	169	16.746	2.558	18.881	1.00	4.89
ATOM	984	CD2	LEU	169	14.864	2.262	20.477	1.00	4.89
ATOM	985	C	LEU	169	12.379	4.759	17.915	1.00	4.07
ATOM	986	O	LEU	169	11.830	5.595	18.634	1.00	4.89
ATOM	987	N	LEU	170	12.373	4.843	16.587	1.00	2.00
ATOM	988	CA	LEU	170	11.834	6.008	15.888	1.00	2.00
ATOM	989	CB	LEU	170	12.027	5.869	14.382	1.00	5.04
ATOM	990	CG	LEU	170	13.257	6.551	13.776	1.00	5.04
ATOM	991	CD1	LEU	170	13.065	8.058	13.715	1.00	5.04
ATOM	992	CD2	LEU	170	14.485	6.194	14.585	1.00	5.04
ATOM	993	C	LEU	170	10.359	6.268	16.198	1.00	2.00
ATOM	994	O	LEU	170	9.949	7.421	16.334	1.00	5.04
ATOM	995	N	TYR	171	9.573	5.205	16.351	1.00	22.09
ATOM	996	CA	TYR	171	8.151	5.340	16.669	1.00	22.09
ATOM	997	CB	TYR	171	7.452	3.981	16.530	1.00	9.28
ATOM	998	CG	TYR	171	6.110	3.846	17.219	1.00	9.28
ATOM	999	CD1	TYR	171	4.939	4.328	16.634	1.00	9.28
ATOM	1000	CE1	TYR	171	3.696	4.181	17.278	1.00	9.28
ATOM	1001	CD2	TYR	171	6.009	3.209	18.460	1.00	9.28

FIG. 3R

ATOM	1002	CE2	TYR	171	4.777	3.063	19.110	1.00	9.28
ATOM	1003	CZ	TYR	171	3.628	3.551	18.515	1.00	9.28
ATOM	1004	OH	TYR	171	2.412	3.411	19.152	1.00	9.28
ATOM	1005	C	TYR	171	7.982	5.915	18.081	1.00	22.09
ATOM	1006	O	TYR	171	7.074	6.717	18.337	1.00	9.28
ATOM	1007	N	GLN	172	8.879	5.529	18.986	1.00	2.00
ATOM	1008	CA	GLN	172	8.830	6.020	20.346	1.00	2.00
ATOM	1009	CB	GLN	172	9.698	5.164	21.251	1.00	13.55
ATOM	1010	CG	GLN	172	9.162	3.775	21.454	1.00	13.55
ATOM	1011	CD	GLN	172	10.033	2.976	22.376	1.00	13.55
ATOM	1012	OE1	GLN	172	9.758	2.867	23.576	1.00	13.55
ATOM	1013	NE2	GLN	172	11.109	2.424	21.834	1.00	13.55
ATOM	1014	C	GLN	172	9.244	7.479	20.411	1.00	2.00
ATOM	1015	O	GLN	172	8.676	8.254	21.183	1.00	13.55
ATOM	1016	N	MET	173	10.202	7.871	19.582	1.00	4.17
ATOM	1017	CA	MET	173	10.642	9.255	19.569	1.00	4.17
ATOM	1018	CB	MET	173	11.800	9.452	18.612	1.00	2.80
ATOM	1019	CG	MET	173	13.130	9.233	19.241	1.00	2.80
ATOM	1020	SD	MET	173	14.412	9.163	18.023	1.00	2.80
ATOM	1021	CE	MET	173	14.864	7.494	18.142	1.00	2.80
ATOM	1022	C	MET	173	9.487	10.128	19.144	1.00	4.17
ATOM	1023	O	MET	173	9.307	11.218	19.672	1.00	2.80
ATOM	1024	N	LEU	174	8.696	9.637	18.195	1.00	6.58
ATOM	1025	CA	LEU	174	7.544	10.387	17.711	1.00	6.58
ATOM	1026	CB	LEU	174	7.069	9.857	16.346	1.00	2.00
ATOM	1027	CG	LEU	174	8.065	9.936	15.177	1.00	2.00
ATOM	1028	CD1	LEU	174	7.532	9.144	13.998	1.00	2.00
ATOM	1029	CD2	LEU	174	8.336	11.393	14.784	1.00	2.00
ATOM	1030	C	LEU	174	6.395	10.426	18.730	1.00	6.58
ATOM	1031	O	LEU	174	5.728	11.456	18.881	1.00	2.00
ATOM	1032	N	CYS	175	6.181	9.332	19.455	1.00	4.87
ATOM	1033	CA	CYS	175	5.118	9.310	20.450	1.00	4.87
ATOM	1034	CB	CYS	175	4.966	7.909	21.033	1.00	2.00
ATOM	1035	SG	CYS	175	4.104	6.748	19.992	1.00	2.00
ATOM	1036	C	CYS	175	5.411	10.321	21.564	1.00	4.87
ATOM	1037	O	CYS	175	4.552	11.119	21.943	1.00	2.00
ATOM	1038	N	GLY	176	6.659	10.315	22.027	1.00	2.00
ATOM	1039	CA	GLY	176	7.093	11.207	23.076	1.00	2.00
ATOM	1040	C	GLY	176	7.004	12.652	22.651	1.00	2.00
ATOM	1041	O	GLY	176	6.575	13.497	23.425	1.00	28.56
ATOM	1042	N	ILE	177	7.373	12.935	21.410	1.00	14.73
ATOM	1043	CA	ILE	177	7.336	14.293	20.882	1.00	14.73
ATOM	1044	CB	ILE	177	8.222	14.419	19.643	1.00	2.00
ATOM	1045	CG2	ILE	177	8.085	15.773	19.020	1.00	2.00
ATOM	1046	CG1	ILE	177	9.676	14.229	20.040	1.00	2.00
ATOM	1047	CD1	ILE	177	10.542	13.878	18.869	1.00	2.00
ATOM	1048	C	ILE	177	5.911	14.721	20.562	1.00	14.73
ATOM	1049	O	ILE	177	5.592	15.908	20.584	1.00	2.00
ATOM	1050	N	LYS	178	5.034	13.758	20.311	1.00	2.00
ATOM	1051	CA	LYS	178	3.659	14.107	20.027	1.00	2.00
ATOM	1052	CB	LYS	178	2.906	12.991	19.310	1.00	12.67
ATOM	1053	CG	LYS	178	1.564	13.501	18.827	1.00	12.67
ATOM	1054	CD	LYS	178	0.546	12.434	18.593	1.00	12.67
ATOM	1055	CE	LYS	178	-0.785	13.112	18.357	1.00	12.67
ATOM	1056	NZ	LYS	178	-1.854	12.145	18.059	1.00	12.67
ATOM	1057	C	LYS	178	2.944	14.456	21.311	1.00	2.00
ATOM	1058	O	LYS	178	2.028	15.263	21.304	1.00	12.67
ATOM	1059	N	HIS	179	3.343	13.833	22.411	1.00	2.00
ATOM	1060	CA	HIS	179	2.729	14.110	23.708	1.00	2.00

FIG. 3S

ATOM	1061	CB	HIS	179	3.168	13.074	24.740	1.00	5.57
ATOM	1062	CG	HIS	179	2.349	13.086	25.993	1.00	5.57
ATOM	1063	CD2	HIS	179	2.678	13.396	27.267	1.00	5.57
ATOM	1064	ND1	HIS	179	1.014	12.743	26.011	1.00	5.57
ATOM	1065	CE1	HIS	179	0.554	12.849	27.243	1.00	5.57
ATOM	1066	NE2	HIS	179	1.545	13.240	28.026	1.00	5.57
ATOM	1067	C	HIS	179	3.178	15.497	24.147	1.00	2.00
ATOM	1068	O	HIS	179	2.405	16.278	24.697	1.00	5.57
ATOM	1069	N	LEU	180	4.437	15.799	23.871	1.00	2.00
ATOM	1070	CA	LEU	180	5.002	17.086	24.193	1.00	2.00
ATOM	1071	CB	LEU	180	6.438	17.165	23.674	1.00	5.28
ATOM	1072	CG	LEU	180	7.537	17.357	24.713	1.00	5.28
ATOM	1073	CD1	LEU	180	7.412	16.299	25.773	1.00	5.28
ATOM	1074	CD2	LEU	180	8.892	17.305	24.063	1.00	5.28
ATOM	1075	C	LEU	180	4.151	18.154	23.509	1.00	2.00
ATOM	1076	O	LEU	180	3.695	19.095	24.143	1.00	5.28
ATOM	1077	N	HIS	181	3.883	17.958	22.225	1.00	2.00
ATOM	1078	CA	HIS	181	3.092	18.901	21.458	1.00	2.00
ATOM	1079	CB	HIS	181	3.194	18.578	19.976	1.00	9.13
ATOM	1080	CG	HIS	181	4.602	18.599	19.449	1.00	9.13
ATOM	1081	CD2	HIS	181	5.768	18.916	20.034	1.00	9.13
ATOM	1082	ND1	HIS	181	4.895	18.279	18.144	1.00	9.13
ATOM	1083	CE1	HIS	181	6.196	18.407	17.950	1.00	9.13
ATOM	1084	NE2	HIS	181	6.752	18.792	19.077	1.00	9.13
ATOM	1085	C	HIS	181	1.626	18.934	21.877	1.00	2.00
ATOM	1086	O	HIS	181	0.941	19.937	21.662	1.00	9.13
ATOM	1087	N	SER	182	1.151	17.857	22.501	1.00	38.18
ATOM	1088	CA	SER	182	-0.235	17.762	22.970	1.00	38.18
ATOM	1089	CB	SER	182	-0.630	16.305	23.248	1.00	31.08
ATOM	1090	OG	SER	182	0.004	15.791	24.408	1.00	31.08
ATOM	1091	C	SER	182	-0.413	18.612	24.227	1.00	38.18
ATOM	1092	O	SER	182	-1.520	19.065	24.534	1.00	31.08
ATOM	1093	N	ALA	183	0.690	18.799	24.951	1.00	14.47
ATOM	1094	CA	ALA	183	0.711	19.609	26.159	1.00	14.47
ATOM	1095	CB	ALA	183	1.670	19.014	27.160	1.00	4.36
ATOM	1096	C	ALA	183	1.104	21.057	25.830	1.00	14.47
ATOM	1097	O	ALA	183	1.148	21.919	26.712	1.00	4.36
ATOM	1098	N	GLY	184	1.382	21.316	24.554	1.00	2.00
ATOM	1099	CA	GLY	184	1.766	22.644	24.113	1.00	2.00
ATOM	1100	C	GLY	184	3.262	22.893	24.181	1.00	2.00
ATOM	1101	O	GLY	184	3.691	24.046	24.081	1.00	17.40
ATOM	1102	N	ILE	185	4.047	21.826	24.370	1.00	2.00
ATOM	1103	CA	ILE	185	5.511	21.894	24.464	1.00	2.00
ATOM	1104	CB	ILE	185	6.041	20.899	25.514	1.00	4.90
ATOM	1105	CG2	ILE	185	7.532	21.128	25.750	1.00	4.90
ATOM	1106	CG1	ILE	185	5.244	21.006	26.808	1.00	4.90
ATOM	1107	CD1	ILE	185	5.464	19.851	27.766	1.00	4.90
ATOM	1108	C	ILE	185	6.205	21.541	23.153	1.00	2.00
ATOM	1109	O	ILE	185	5.973	20.468	22.613	1.00	4.90
ATOM	1110	N	ILE	186	7.077	22.423	22.666	1.00	7.82
ATOM	1111	CA	ILE	186	7.823	22.185	21.428	1.00	7.82
ATOM	1112	CB	ILE	186	7.435	23.175	20.302	1.00	17.50
ATOM	1113	CG2	ILE	186	8.323	22.972	19.099	1.00	17.50
ATOM	1114	CG1	ILE	186	5.983	22.934	19.882	1.00	17.50
ATOM	1115	CD1	ILE	186	5.434	23.973	18.961	1.00	17.50
ATOM	1116	C	ILE	186	9.326	22.221	21.688	1.00	7.82
ATOM	1117	O	ILE	186	9.962	23.267	21.659	1.00	17.50
ATOM	1118	N	HIS	187	9.872	21.023	21.849	1.00	22.00
ATOM	1119	CA	HIS	187	11.277	20.752	22.148	1.00	22.00

FIG. 3T

ATOM	1120	CB	HIS	187	11.575	19.297	21.774	1.00	3.84
ATOM	1121	CG	HIS	187	12.554	18.623	22.682	1.00	3.84
ATOM	1122	CD2	HIS	187	12.384	17.652	23.602	1.00	3.84
ATOM	1123	ND1	HIS	187	13.895	18.941	22.699	1.00	3.84
ATOM	1124	CE1	HIS	187	14.509	18.191	23.594	1.00	3.84
ATOM	1125	NE2	HIS	187	13.614	17.400	24.157	1.00	3.84
ATOM	1126	C	HIS	187	12.310	21.680	21.518	1.00	22.00
ATOM	1127	O	HIS	187	12.891	22.526	22.197	1.00	3.84
ATOM	1128	N	ARG	188	12.508	21.499	20.216	1.00	6.22
ATOM	1129	CA	ARG	188	13.463	22.242	19.401	1.00	6.22
ATOM	1130	CB	ARG	188	13.201	23.739	19.445	1.00	27.37
ATOM	1131	CG	ARG	188	11.932	24.159	18.755	1.00	27.37
ATOM	1132	CD	ARG	188	11.856	25.658	18.715	1.00	27.37
ATOM	1133	NE	ARG	188	11.646	26.237	20.043	1.00	27.37
ATOM	1134	CZ	ARG	188	12.366	27.234	20.560	1.00	27.37
ATOM	1135	NH1	ARG	188	13.368	27.775	19.875	1.00	27.37
ATOM	1136	NH2	ARG	188	12.038	27.749	21.742	1.00	27.37
ATOM	1137	C	ARG	188	14.944	21.950	19.652	1.00	6.22
ATOM	1138	O	ARG	188	15.799	22.651	19.123	1.00	27.37
ATOM	1139	N	ASP	189	15.250	20.919	20.445	1.00	12.44
ATOM	1140	CA	ASP	189	16.646	20.543	20.705	1.00	12.44
ATOM	1141	CB	ASP	189	17.240	21.367	21.859	1.00	15.30
ATOM	1142	CG	ASP	189	18.767	21.294	21.907	1.00	15.30
ATOM	1143	OD1	ASP	189	19.413	21.349	20.835	1.00	15.30
ATOM	1144	OD2	ASP	189	19.320	21.164	23.017	1.00	15.30
ATOM	1145	C	ASP	189	16.879	19.035	20.933	1.00	12.44
ATOM	1146	O	ASP	189	17.730	18.635	21.731	1.00	15.30
ATOM	1147	N	LEU	190	16.139	18.202	20.208	1.00	2.00
ATOM	1148	CA	LEU	190	16.293	16.757	20.327	1.00	2.00
ATOM	1149	CB	LEU	190	15.263	16.035	19.467	1.00	11.08
ATOM	1150	CG	LEU	190	13.848	16.009	20.029	1.00	11.08
ATOM	1151	CD1	LEU	190	12.872	16.076	18.889	1.00	11.08
ATOM	1152	CD2	LEU	190	13.618	14.777	20.900	1.00	11.08
ATOM	1153	C	LEU	190	17.680	16.353	19.860	1.00	2.00
ATOM	1154	O	LEU	190	18.072	16.672	18.755	1.00	11.08
ATOM	1155	N	LYS	191	18.432	15.680	20.715	1.00	2.00
ATOM	1156	CA	LYS	191	19.764	15.222	20.357	1.00	2.00
ATOM	1157	CB	LYS	191	20.829	16.200	20.852	1.00	15.76
ATOM	1158	CG	LYS	191	20.620	16.731	22.261	1.00	15.76
ATOM	1159	CD	LYS	191	21.700	17.727	22.660	1.00	15.76
ATOM	1160	CE	LYS	191	21.478	19.088	22.025	1.00	15.76
ATOM	1161	NZ	LYS	191	22.411	20.123	22.562	1.00	15.76
ATOM	1162	C	LYS	191	19.932	13.829	20.941	1.00	2.00
ATOM	1163	O	LYS	191	19.342	13.518	21.954	1.00	15.76
ATOM	1164	N	PRO	192	20.669	12.944	20.259	1.00	8.42
ATOM	1165	CD	PRO	192	21.359	13.131	18.973	1.00	6.93
ATOM	1166	CA	PRO	192	20.872	11.579	20.756	1.00	8.42
ATOM	1167	CB	PRO	192	21.939	11.032	19.809	1.00	6.93
ATOM	1168	CG	PRO	192	21.594	11.704	18.522	1.00	6.93
ATOM	1169	C	PRO	192	21.318	11.529	22.205	1.00	8.42
ATOM	1170	O	PRO	192	20.848	10.697	22.985	1.00	6.93
ATOM	1171	N	SER	193	22.190	12.464	22.576	1.00	15.86
ATOM	1172	CA	SER	193	22.699	12.527	23.935	1.00	15.86
ATOM	1173	CB	SER	193	23.830	13.569	24.063	1.00	24.60
ATOM	1174	OG	SER	193	23.439	14.886	23.709	1.00	24.60
ATOM	1175	C	SER	193	21.582	12.804	24.931	1.00	15.86
ATOM	1176	O	SER	193	21.705	12.459	26.101	1.00	24.60
ATOM	1177	N	ASN	194	20.475	13.372	24.453	1.00	5.51
ATOM	1178	CA	ASN	194	19.327	13.685	25.306	1.00	5.51

FIG. 3U

ATOM	1179	CB	ASN	194	18.844	15.115	25.057	1.00	7.93
ATOM	1180	CG	ASN	194	19.824	16.151	25.558	1.00	7.93
ATOM	1181	OD1	ASN	194	20.810	15.821	26.222	1.00	7.93
ATOM	1182	ND2	ASN	194	19.567	17.406	25.251	1.00	7.93
ATOM	1183	C	ASN	194	18.173	12.701	25.156	1.00	5.51
ATOM	1184	O	ASN	194	17.006	13.050	25.369	1.00	7.93
ATOM	1185	N	ILE	195	18.509	11.487	24.738	1.00	2.00
ATOM	1186	CA	ILE	195	17.549	10.414	24.570	1.00	2.00
ATOM	1187	CB	ILE	195	17.168	10.196	23.094	1.00	11.94
ATOM	1188	CG2	ILE	195	16.066	9.167	23.015	1.00	11.94
ATOM	1189	CG1	ILE	195	16.701	11.496	22.446	1.00	11.94
ATOM	1190	CD1	ILE	195	16.189	11.344	21.041	1.00	11.94
ATOM	1191	C	ILE	195	18.260	9.174	25.074	1.00	2.00
ATOM	1192	O	ILE	195	19.418	8.931	24.738	1.00	11.94
ATOM	1193	N	VAL	196	17.584	8.402	25.909	1.00	2.00
ATOM	1194	CA	VAL	196	18.175	7.192	26.463	1.00	2.00
ATOM	1195	CB	VAL	196	18.364	7.288	28.004	1.00	2.00
ATOM	1196	CG1	VAL	196	19.559	8.175	28.334	1.00	2.00
ATOM	1197	CG2	VAL	196	17.104	7.831	28.680	1.00	2.00
ATOM	1198	C	VAL	196	17.379	5.948	26.100	1.00	2.00
ATOM	1199	O	VAL	196	16.164	6.010	25.887	1.00	2.00
ATOM	1200	N	VAL	197	18.083	4.816	26.018	1.00	25.26
ATOM	1201	CA	VAL	197	17.466	3.529	25.669	1.00	25.26
ATOM	1202	CB	VAL	197	17.871	3.056	24.250	1.00	3.01
ATOM	1203	CG1	VAL	197	17.301	3.987	23.196	1.00	3.01
ATOM	1204	CG2	VAL	197	19.386	2.944	24.131	1.00	3.01
ATOM	1205	C	VAL	197	17.711	2.382	26.652	1.00	25.26
ATOM	1206	O	VAL	197	18.615	2.422	27.492	1.00	3.01
ATOM	1207	N	LYS	198	16.841	1.382	26.563	1.00	8.42
ATOM	1208	CA	LYS	198	16.924	0.191	27.393	1.00	8.42
ATOM	1209	CB	LYS	198	15.583	-0.091	28.070	1.00	30.51
ATOM	1210	CG	LYS	198	15.690	-0.379	29.574	1.00	30.51
ATOM	1211	CD	LYS	198	14.314	-0.471	30.219	1.00	30.51
ATOM	1212	CE	LYS	198	13.538	0.837	30.039	1.00	30.51
ATOM	1213	NZ	LYS	198	12.062	0.708	30.271	1.00	30.51
ATOM	1214	C	LYS	198	17.305	-0.950	26.462	1.00	8.42
ATOM	1215	O	LYS	198	17.233	-0.812	25.238	1.00	30.51
ATOM	1216	N	SER	199	17.688	-2.082	27.041	1.00	12.70
ATOM	1217	CA	SER	199	18.096	-3.247	26.260	1.00	12.70
ATOM	1218	CB	SER	199	18.808	-4.261	27.154	1.00	2.13
ATOM	1219	OG	SER	199	20.040	-3.730	27.628	1.00	2.13
ATOM	1220	C	SER	199	16.929	-3.898	25.518	1.00	12.70
ATOM	1221	O	SER	199	17.110	-4.445	24.440	1.00	2.13
ATOM	1222	N	ASP	200	15.730	-3.795	26.091	1.00	2.00
ATOM	1223	CA	ASP	200	14.526	-4.362	25.484	1.00	2.00
ATOM	1224	CB	ASP	200	13.440	-4.653	26.536	1.00	13.93
ATOM	1225	CG	ASP	200	12.980	-3.410	27.300	1.00	13.93
ATOM	1226	OD1	ASP	200	12.159	-3.554	28.228	1.00	13.93
ATOM	1227	OD2	ASP	200	13.434	-2.294	26.997	1.00	13.93
ATOM	1228	C	ASP	200	13.968	-3.444	24.424	1.00	2.00
ATOM	1229	O	ASP	200	12.801	-3.553	24.054	1.00	13.93
ATOM	1230	N	CYS	201	14.794	-2.475	24.027	1.00	34.23
ATOM	1231	CA	CYS	201	14.459	-1.494	23.002	1.00	34.23
ATOM	1232	CB	CYS	201	14.047	-2.221	21.712	1.00	23.39
ATOM	1233	SG	CYS	201	14.806	-1.561	20.216	1.00	23.39
ATOM	1234	C	CYS	201	13.427	-0.417	23.384	1.00	34.23
ATOM	1235	O	CYS	201	12.812	0.196	22.521	1.00	23.39
ATOM	1236	N	THR	202	13.205	-0.203	24.671	1.00	5.40
ATOM	1237	CA	THR	202	12.267	0.841	25.065	1.00	5.40

FIG. 3V

ATOM	1238	CB	THR	202	11.569	0.533	26.393	1.00	3.53
ATOM	1239	OG1	THR	202	12.519	0.015	27.325	1.00	3.53
ATOM	1240	CG2	THR	202	10.450	-0.470	26.181	1.00	3.53
ATOM	1241	C	THR	202	13.026	2.154	25.122	1.00	5.40
ATOM	1242	O	THR	202	14.192	2.184	25.519	1.00	3.53
ATOM	1243	N	LEU	203	12.375	3.231	24.696	1.00	6.11
ATOM	1244	CA	LEU	203	13.022	4.537	24.641	1.00	6.11
ATOM	1245	CB	LEU	203	13.267	4.898	23.160	1.00	2.00
ATOM	1246	CG	LEU	203	13.898	6.228	22.739	1.00	2.00
ATOM	1247	CD1	LEU	203	14.745	6.067	21.485	1.00	2.00
ATOM	1248	CD2	LEU	203	12.805	7.260	22.537	1.00	2.00
ATOM	1249	C	LEU	203	12.318	5.678	25.384	1.00	6.11
ATOM	1250	O	LEU	203	11.093	5.743	25.440	1.00	2.00
ATOM	1251	N	LYS	204	13.126	6.580	25.943	1.00	2.00
ATOM	1252	CA	LYS	204	12.640	7.749	26.679	1.00	2.00
ATOM	1253	CB	LYS	204	12.649	7.484	28.189	1.00	15.81
ATOM	1254	CG	LYS	204	11.461	6.691	28.713	1.00	15.81
ATOM	1255	CD	LYS	204	11.669	6.344	30.176	1.00	15.81
ATOM	1256	CE	LYS	204	10.467	5.612	30.739	1.00	15.81
ATOM	1257	NZ	LYS	204	9.735	6.418	31.772	1.00	15.81
ATOM	1258	C	LYS	204	13.473	9.003	26.386	1.00	2.00
ATOM	1259	O	LYS	204	14.664	8.929	26.077	1.00	15.81
ATOM	1260	N	ILE	205	12.822	10.155	26.457	1.00	2.00
ATOM	1261	CA	ILE	205	13.467	11.437	26.222	1.00	2.00
ATOM	1262	CB	ILE	205	12.566	12.327	25.335	1.00	4.27
ATOM	1263	CG2	ILE	205	13.193	13.713	25.165	1.00	4.27
ATOM	1264	CG1	ILE	205	12.375	11.623	23.978	1.00	4.27
ATOM	1265	CD1	ILE	205	11.334	12.228	23.067	1.00	4.27
ATOM	1266	C	ILE	205	13.746	12.082	27.578	1.00	2.00
ATOM	1267	O	ILE	205	12.885	12.099	28.454	1.00	4.27
ATOM	1268	N	LEU	206	14.966	12.590	27.744	1.00	9.54
ATOM	1269	CA	LEU	206	15.401	13.212	28.995	1.00	9.54
ATOM	1270	CB	LEU	206	16.916	13.070	29.149	1.00	2.00
ATOM	1271	CG	LEU	206	17.509	11.665	29.133	1.00	2.00
ATOM	1272	CD1	LEU	206	19.016	11.740	29.282	1.00	2.00
ATOM	1273	CD2	LEU	206	16.895	10.831	30.240	1.00	2.00
ATOM	1274	C	LEU	206	14.975	14.669	29.236	1.00	9.54
ATOM	1275	O	LEU	206	14.370	14.961	30.265	1.00	2.00
ATOM	1276	N	ASP	207	15.279	15.568	28.298	1.00	2.00
ATOM	1277	CA	ASP	207	14.922	16.984	28.433	1.00	2.00
ATOM	1278	CB	ASP	207	16.142	17.877	28.130	1.00	21.09
ATOM	1279	CG	ASP	207	16.622	17.795	26.672	1.00	21.09
ATOM	1280	OD1	ASP	207	16.316	16.816	25.946	1.00	21.09
ATOM	1281	OD2	ASP	207	17.334	18.734	26.248	1.00	21.09
ATOM	1282	C	ASP	207	13.694	17.442	27.628	1.00	2.00
ATOM	1283	O	ASP	207	13.144	16.682	26.834	1.00	21.09
ATOM	1284	N	PHE	208	13.258	18.680	27.872	1.00	10.73
ATOM	1285	CA	PHE	208	12.107	19.280	27.180	1.00	10.73
ATOM	1286	CB	PHE	208	11.056	19.774	28.182	1.00	2.16
ATOM	1287	CG	PHE	208	10.493	18.678	29.054	1.00	2.16
ATOM	1288	CD1	PHE	208	11.197	18.236	30.183	1.00	2.16
ATOM	1289	CD2	PHE	208	9.297	18.052	28.720	1.00	2.16
ATOM	1290	CE1	PHE	208	10.727	17.173	30.968	1.00	2.16
ATOM	1291	CE2	PHE	208	8.809	16.986	29.493	1.00	2.16
ATOM	1292	CZ	PHE	208	9.528	16.539	30.622	1.00	2.16
ATOM	1293	C	PHE	208	12.592	20.403	26.268	1.00	10.73
ATOM	1294	O	PHE	208	11.814	21.161	25.688	1.00	2.16
ATOM	1295	N	GLY	209	13.915	20.484	26.177	1.00	5.67
ATOM	1296	CA	GLY	209	14.591	21.435	25.325	1.00	5.67

FIG. 3W

ATOM	1297	C	GLY	209	14.420	22.917	25.544	1.00	5.67
ATOM	1298	O	GLY	209	14.431	23.427	26.673	1.00	33.44
ATOM	1299	N	LEU	210	14.299	23.604	24.413	1.00	21.09
ATOM	1300	CA	LEU	210	14.155	25.052	24.363	1.00	21.09
ATOM	1301	CB	LEU	210	14.411	25.531	22.928	1.00	15.39
ATOM	1302	CG	LEU	210	15.869	25.761	22.500	1.00	15.39
ATOM	1303	CD1	LEU	210	16.791	24.688	23.048	1.00	15.39
ATOM	1304	CD2	LEU	210	15.967	25.854	20.987	1.00	15.39
ATOM	1305	C	LEU	210	12.806	25.553	24.868	1.00	21.09
ATOM	1306	O	LEU	210	11.781	24.872	24.740	1.00	15.39
ATOM	1307	N	ALA	211	12.825	26.740	25.466	1.00	12.93
ATOM	1308	CA	ALA	211	11.616	27.358	25.993	1.00	12.93
ATOM	1309	CB	ALA	211	11.970	28.365	27.092	1.00	26.16
ATOM	1310	C	ALA	211	10.851	28.049	24.873	1.00	12.93
ATOM	1311	O	ALA	211	11.504	28.842	24.167	1.00	26.16
ATOM	1312	CB	THR	217	20.244	32.345	26.028	1.00	51.78
ATOM	1313	OG1	THR	217	20.882	31.058	26.017	1.00	51.78
ATOM	1314	CG2	THR	217	20.335	32.984	24.649	1.00	51.78
ATOM	1315	C	THR	217	22.426	33.123	27.062	1.00	44.85
ATOM	1316	O	THR	217	23.008	32.685	26.058	1.00	51.78
ATOM	1317	N	THR	217	20.488	34.675	26.939	1.00	44.85
ATOM	1318	CA	THR	217	20.902	33.255	27.103	1.00	44.85
ATOM	1319	N	PHE	218	23.063	33.473	28.176	1.00	53.03
ATOM	1320	CA	PHE	218	24.512	33.400	28.273	1.00	53.03
ATOM	1321	CB	PHE	218	25.091	34.820	28.360	1.00	30.03
ATOM	1322	CG	PHE	218	26.582	34.867	28.555	1.00	30.03
ATOM	1323	CD1	PHE	218	27.446	34.687	27.474	1.00	30.03
ATOM	1324	CD2	PHE	218	27.121	35.110	29.820	1.00	30.03
ATOM	1325	CE1	PHE	218	28.833	34.748	27.644	1.00	30.03
ATOM	1326	CE2	PHE	218	28.509	35.174	30.014	1.00	30.03
ATOM	1327	CZ	PHE	218	29.374	34.992	28.919	1.00	30.03
ATOM	1328	C	PHE	218	24.960	32.523	29.453	1.00	53.03
ATOM	1329	O	PHE	218	24.265	32.409	30.478	1.00	30.03
ATOM	1330	N	MET	219	26.104	31.871	29.261	1.00	33.01
ATOM	1331	CA	MET	219	26.713	30.992	30.251	1.00	33.01
ATOM	1332	CB	MET	219	26.383	29.529	29.945	1.00	57.60
ATOM	1333	CG	MET	219	25.102	28.960	30.517	1.00	57.60
ATOM	1334	SD	MET	219	25.090	27.161	30.128	1.00	57.60
ATOM	1335	CE	MET	219	24.715	27.219	28.251	1.00	57.60
ATOM	1336	C	MET	219	28.215	31.132	30.085	1.00	33.01
ATOM	1337	O	MET	219	28.694	31.476	29.001	1.00	57.60
ATOM	1338	N	MET	220	28.962	30.879	31.154	1.00	36.45
ATOM	1339	CA	MET	220	30.408	30.920	31.035	1.00	36.45
ATOM	1340	CB	MET	220	31.052	31.852	32.063	1.00	15.11
ATOM	1341	CG	MET	220	31.584	33.117	31.410	1.00	15.11
ATOM	1342	SD	MET	220	32.595	34.145	32.466	1.00	15.11
ATOM	1343	CE	MET	220	31.381	35.216	33.043	1.00	15.11
ATOM	1344	C	MET	220	30.983	29.497	31.070	1.00	36.45
ATOM	1345	O	MET	220	32.078	29.255	31.590	1.00	15.11
ATOM	1346	N	THR	221	30.234	28.568	30.473	1.00	39.69
ATOM	1347	CA	THR	221	30.647	27.170	30.381	1.00	39.69
ATOM	1348	CB	THR	221	29.474	26.227	29.943	1.00	47.10
ATOM	1349	OG1	THR	221	28.223	26.714	30.453	1.00	47.10
ATOM	1350	CG2	THR	221	29.705	24.804	30.474	1.00	47.10
ATOM	1351	C	THR	221	31.756	27.079	29.322	1.00	39.69
ATOM	1352	O	THR	221	31.746	27.911	28.377	1.00	47.10
ATOM	1353	CB	VAL	224	30.615	23.807	22.560	1.00	24.68
ATOM	1354	CG1	VAL	224	30.847	22.384	22.022	1.00	24.68
ATOM	1355	CG2	VAL	224	29.898	24.679	21.524	1.00	24.68

FIG. 3X

ATOM	1356	C	VAL	224	28.536	22.979	23.715	1.00	32.19
ATOM	1357	O	VAL	224	28.480	21.788	24.050	1.00	24.68
ATOM	1358	N	VAL	224	30.614	23.160	25.007	1.00	32.19
ATOM	1359	CA	VAL	224	29.818	23.776	23.904	1.00	32.19
ATOM	1360	N	VAL	225	27.504	23.661	23.220	1.00	31.51
ATOM	1361	CA	VAL	225	26.195	23.055	22.963	1.00	31.51
ATOM	1362	CB	VAL	225	25.057	24.106	23.005	1.00	14.81
ATOM	1363	CG1	VAL	225	23.715	23.408	23.114	1.00	14.81
ATOM	1364	CG2	VAL	225	25.258	25.091	24.153	1.00	14.81
ATOM	1365	C	VAL	225	26.178	22.405	21.578	1.00	31.51
ATOM	1366	O	VAL	225	26.782	22.923	20.630	1.00	14.81
ATOM	1367	N	THR	226	25.475	21.279	21.466	1.00	28.04
ATOM	1368	CA	THR	226	25.375	20.564	20.198	1.00	28.04
ATOM	1369	CB	THR	226	25.213	19.042	20.412	1.00	35.95
ATOM	1370	OG1	THR	226	26.259	18.568	21.278	1.00	35.95
ATOM	1371	CG2	THR	226	25.305	18.308	19.069	1.00	35.95
ATOM	1372	C	THR	226	24.206	21.128	19.390	1.00	28.04
ATOM	1373	O	THR	226	23.057	21.100	19.831	1.00	35.95
ATOM	1374	N	ARG	227	24.511	21.597	18.184	1.00	20.49
ATOM	1375	CA	ARG	227	23.518	22.220	17.320	1.00	20.49
ATOM	1376	CB	ARG	227	24.025	23.611	16.944	1.00	27.34
ATOM	1377	CG	ARG	227	25.440	23.563	16.354	1.00	27.34
ATOM	1378	CD	ARG	227	26.164	24.869	16.543	1.00	27.34
ATOM	1379	NE	ARG	227	25.948	25.423	17.877	1.00	27.34
ATOM	1380	CZ	ARG	227	25.822	26.721	18.134	1.00	27.34
ATOM	1381	NH1	ARG	227	25.902	27.605	17.149	1.00	27.34
ATOM	1382	NH2	ARG	227	25.567	27.140	19.370	1.00	27.34
ATOM	1383	C	ARG	227	23.236	21.450	16.041	1.00	20.49
ATOM	1384	O	ARG	227	22.315	21.793	15.293	1.00	27.34
ATOM	1385	N	TYR	228	24.020	20.410	15.803	1.00	2.02
ATOM	1386	CA	TYR	228	23.890	19.634	14.584	1.00	2.02
ATOM	1387	CB	TYR	228	24.819	18.421	14.624	1.00	15.88
ATOM	1388	CG	TYR	228	26.211	18.676	15.146	1.00	15.88
ATOM	1389	CD1	TYR	228	26.807	19.926	15.055	1.00	15.88
ATOM	1390	CE1	TYR	228	28.102	20.141	15.518	1.00	15.88
ATOM	1391	CD2	TYR	228	26.945	17.651	15.713	1.00	15.88
ATOM	1392	CE2	TYR	228	28.233	17.854	16.171	1.00	15.88
ATOM	1393	CZ	TYR	228	28.808	19.095	16.075	1.00	15.88
ATOM	1394	OH	TYR	228	30.087	19.273	16.550	1.00	15.88
ATOM	1395	C	TYR	228	22.482	19.151	14.242	1.00	2.02
ATOM	1396	O	TYR	228	22.194	18.887	13.081	1.00	15.88
ATOM	1397	N	TYR	229	21.597	19.060	15.229	1.00	16.06
ATOM	1398	CA	TYR	229	20.248	18.540	14.976	1.00	16.06
ATOM	1399	CB	TYR	229	19.909	17.421	15.992	1.00	7.45
ATOM	1400	CG	TYR	229	21.065	16.473	16.273	1.00	7.45
ATOM	1401	CD1	TYR	229	22.113	16.850	17.116	1.00	7.45
ATOM	1402	CE1	TYR	229	23.219	16.033	17.305	1.00	7.45
ATOM	1403	CD2	TYR	229	21.155	15.231	15.641	1.00	7.45
ATOM	1404	CE2	TYR	229	22.266	14.406	15.833	1.00	7.45
ATOM	1405	CZ	TYR	229	23.292	14.822	16.663	1.00	7.45
ATOM	1406	OH	TYR	229	24.428	14.074	16.824	1.00	7.45
ATOM	1407	C	TYR	229	19.159	19.609	14.962	1.00	16.06
ATOM	1408	O	TYR	229	17.972	19.317	15.126	1.00	7.45
ATOM	1409	N	ARG	230	19.559	20.845	14.698	1.00	14.21
ATOM	1410	CA	ARG	230	18.604	21.945	14.681	1.00	14.21
ATOM	1411	CB	ARG	230	19.234	23.218	15.249	1.00	40.21
ATOM	1412	CG	ARG	230	19.643	23.088	16.726	1.00	40.21
ATOM	1413	CD	ARG	230	19.970	24.444	17.327	1.00	40.21
ATOM	1414	NE	ARG	230	20.596	24.378	18.650	1.00	40.21

FIG. 3Y

ATOM	1415	CZ	ARG	230	19.948	24.518	19.802	1.00	40.21
ATOM	1416	NH1	ARG	230	18.635	24.720	19.805	1.00	40.21
ATOM	1417	NH2	ARG	230	20.624	24.522	20.950	1.00	40.21
ATOM	1418	C	ARG	230	17.996	22.210	13.311	1.00	14.21
ATOM	1419	O	ARG	230	18.669	22.095	12.283	1.00	40.21
ATOM	1420	N	ALA	231	16.715	22.570	13.317	1.00	2.00
ATOM	1421	CA	ALA	231	15.966	22.843	12.097	1.00	2.00
ATOM	1422	CB	ALA	231	14.489	22.874	12.386	1.00	3.97
ATOM	1423	C	ALA	231	16.423	24.164	11.494	1.00	2.00
ATOM	1424	O	ALA	231	17.041	24.978	12.170	1.00	3.97
ATOM	1425	N	PRO	232	16.145	24.391	10.202	1.00	19.85
ATOM	1426	CD	PRO	232	15.491	23.457	9.272	1.00	34.15
ATOM	1427	CA	PRO	232	16.529	25.618	9.494	1.00	19.85
ATOM	1428	CB	PRO	232	16.128	25.306	8.041	1.00	34.15
ATOM	1429	CG	PRO	232	16.156	23.797	7.967	1.00	34.15
ATOM	1430	C	PRO	232	15.756	26.809	10.018	1.00	19.85
ATOM	1431	O	PRO	232	16.247	27.936	10.034	1.00	34.15
ATOM	1432	N	GLU	233	14.532	26.539	10.453	1.00	5.93
ATOM	1433	CA	GLU	233	13.657	27.567	10.984	1.00	5.93
ATOM	1434	CB	GLU	233	12.210	27.056	11.092	1.00	20.38
ATOM	1435	CG	GLU	233	12.010	25.814	11.959	1.00	20.38
ATOM	1436	CD	GLU	233	11.421	24.626	11.190	1.00	20.38
ATOM	1437	OE1	GLU	233	12.204	23.889	10.554	1.00	20.38
ATOM	1438	OE2	GLU	233	10.181	24.432	11.234	1.00	20.38
ATOM	1439	C	GLU	233	14.164	28.053	12.333	1.00	5.93
ATOM	1440	O	GLU	233	13.616	29.000	12.909	1.00	20.38
ATOM	1441	N	VAL	234	15.222	27.404	12.820	1.00	2.00
ATOM	1442	CA	VAL	234	15.855	27.745	14.079	1.00	2.00
ATOM	1443	CB	VAL	234	15.972	26.501	15.002	1.00	7.29
ATOM	1444	CG1	VAL	234	17.045	26.718	16.071	1.00	7.29
ATOM	1445	CG2	VAL	234	14.620	26.203	15.671	1.00	7.29
ATOM	1446	C	VAL	234	17.253	28.275	13.769	1.00	2.00
ATOM	1447	O	VAL	234	17.700	29.254	14.353	1.00	7.29
ATOM	1448	N	ILE	235	17.936	27.632	12.833	1.00	32.07
ATOM	1449	CA	ILE	235	19.272	28.046	12.433	1.00	32.07
ATOM	1450	CB	ILE	235	19.878	27.013	11.476	1.00	7.32
ATOM	1451	CG2	ILE	235	21.224	27.486	10.939	1.00	7.32
ATOM	1452	CG1	ILE	235	20.041	25.692	12.229	1.00	7.32
ATOM	1453	CD1	ILE	235	20.523	24.554	11.381	1.00	7.32
ATOM	1454	C	ILE	235	19.236	29.422	11.784	1.00	32.07
ATOM	1455	O	ILE	235	20.216	30.166	11.832	1.00	7.32
ATOM	1456	N	LEU	236	18.088	29.759	11.199	1.00	29.90
ATOM	1457	CA	LEU	236	17.893	31.043	10.535	1.00	29.90
ATOM	1458	CB	LEU	236	17.501	30.818	9.081	1.00	2.52
ATOM	1459	CG	LEU	236	18.477	29.992	8.248	1.00	2.52
ATOM	1460	CD1	LEU	236	17.772	29.595	6.969	1.00	2.52
ATOM	1461	CD2	LEU	236	19.779	30.747	7.965	1.00	2.52
ATOM	1462	C	LEU	236	16.810	31.850	11.244	1.00	29.90
ATOM	1463	O	LEU	236	16.445	32.941	10.808	1.00	2.52
ATOM	1464	N	GLY	237	16.267	31.262	12.308	1.00	27.32
ATOM	1465	CA	GLY	237	15.236	31.887	13.117	1.00	27.32
ATOM	1466	C	GLY	237	14.135	32.598	12.360	1.00	27.32
ATOM	1467	O	GLY	237	14.138	33.829	12.270	1.00	32.38
ATOM	1468	N	MET	238	13.193	31.831	11.813	1.00	36.62
ATOM	1469	CA	MET	238	12.087	32.411	11.064	1.00	36.62
ATOM	1470	CB	MET	238	12.134	31.908	9.627	1.00	19.68
ATOM	1471	CG	MET	238	11.861	30.433	9.478	1.00	19.68
ATOM	1472	SD	MET	238	12.644	29.863	7.990	1.00	19.68
ATOM	1473	CE	MET	238	14.336	29.930	8.549	1.00	19.68

FIG. 3Z

ATOM	1474	C	MET	238	10.718	32.091	11.662	1.00	36.62
ATOM	1475	O	MET	238	9.679	32.428	11.076	1.00	19.68
ATOM	1476	N	GLY	239	10.718	31.487	12.844	1.00	3.52
ATOM	1477	CA	GLY	239	9.470	31.105	13.472	1.00	3.52
ATOM	1478	C	GLY	239	9.390	29.604	13.327	1.00	3.52
ATOM	1479	O	GLY	239	10.337	28.988	12.832	1.00	6.91
ATOM	1480	N	TYR	240	8.294	28.998	13.773	1.00	2.00
ATOM	1481	CA	TYR	240	8.168	27.546	13.686	1.00	2.00
ATOM	1482	CB	TYR	240	9.241	26.864	14.570	1.00	15.34
ATOM	1483	CG	TYR	240	9.198	27.170	16.070	1.00	15.34
ATOM	1484	CD1	TYR	240	8.368	26.452	16.932	1.00	15.34
ATOM	1485	CE1	TYR	240	8.326	26.731	18.303	1.00	15.34
ATOM	1486	CD2	TYR	240	9.992	28.178	16.626	1.00	15.34
ATOM	1487	CE2	TYR	240	9.954	28.466	17.997	1.00	15.34
ATOM	1488	CZ	TYR	240	9.117	27.740	18.825	1.00	15.34
ATOM	1489	OH	TYR	240	9.049	28.041	20.164	1.00	15.34
ATOM	1490	C	TYR	240	6.802	27.005	14.070	1.00	2.00
ATOM	1491	O	TYR	240	5.915	27.751	14.481	1.00	15.34
ATOM	1492	N	LYS	241	6.626	25.704	13.888	1.00	2.00
ATOM	1493	CA	LYS	241	5.406	25.036	14.298	1.00	2.00
ATOM	1494	CB	LYS	241	4.376	24.928	13.166	1.00	9.47
ATOM	1495	CG	LYS	241	4.863	24.349	11.851	1.00	9.47
ATOM	1496	CD	LYS	241	3.667	24.134	10.930	1.00	9.47
ATOM	1497	CE	LYS	241	4.050	23.720	9.511	1.00	9.47
ATOM	1498	NZ	LYS	241	2.830	23.442	8.669	1.00	9.47
ATOM	1499	C	LYS	241	5.789	23.682	14.900	1.00	2.00
ATOM	1500	O	LYS	241	6.960	23.436	15.184	1.00	9.47
ATOM	1501	N	GLU	242	4.811	22.818	15.128	1.00	3.20
ATOM	1502	CA	GLU	242	5.065	21.503	15.720	1.00	3.20
ATOM	1503	CB	GLU	242	3.767	20.703	15.885	1.00	26.25
ATOM	1504	CG	GLU	242	2.465	21.471	15.649	1.00	26.25
ATOM	1505	CD	GLU	242	2.189	22.526	16.708	1.00	26.25
ATOM	1506	OE1	GLU	242	1.730	22.153	17.820	1.00	26.25
ATOM	1507	OE2	GLU	242	2.414	23.727	16.410	1.00	26.25
ATOM	1508	C	GLU	242	6.054	20.642	14.946	1.00	3.20
ATOM	1509	O	GLU	242	6.743	19.818	15.539	1.00	26.25
ATOM	1510	N	ASN	243	6.106	20.812	13.629	1.00	11.35
ATOM	1511	CA	ASN	243	7.002	20.013	12.799	1.00	11.35
ATOM	1512	CB	ASN	243	6.471	19.940	11.356	1.00	19.67
ATOM	1513	CG	ASN	243	6.636	21.251	10.578	1.00	19.67
ATOM	1514	OD1	ASN	243	7.122	22.261	11.098	1.00	19.67
ATOM	1515	ND2	ASN	243	6.253	21.219	9.312	1.00	19.67
ATOM	1516	C	ASN	243	8.482	20.409	12.805	1.00	11.35
ATOM	1517	O	ASN	243	9.248	19.919	11.989	1.00	19.67
ATOM	1518	N	VAL	244	8.890	21.293	13.707	1.00	6.71
ATOM	1519	CA	VAL	244	10.291	21.688	13.785	1.00	6.71
ATOM	1520	CB	VAL	244	10.478	23.032	14.569	1.00	2.00
ATOM	1521	CG1	VAL	244	9.830	22.954	15.941	1.00	2.00
ATOM	1522	CG2	VAL	244	11.958	23.406	14.676	1.00	2.00
ATOM	1523	C	VAL	244	11.133	20.570	14.411	1.00	6.71
ATOM	1524	O	VAL	244	12.359	20.532	14.265	1.00	2.00
ATOM	1525	N	ASP	245	10.470	19.650	15.103	1.00	6.59
ATOM	1526	CA	ASP	245	11.154	18.527	15.738	1.00	6.59
ATOM	1527	CB	ASP	245	10.385	18.096	16.988	1.00	3.97
ATOM	1528	CG	ASP	245	10.553	19.059	18.151	1.00	3.97
ATOM	1529	OD1	ASP	245	11.703	19.434	18.438	1.00	3.97
ATOM	1530	OD2	ASP	245	9.542	19.415	18.780	1.00	3.97
ATOM	1531	C	ASP	245	11.327	17.344	14.773	1.00	6.59
ATOM	1532	O	ASP	245	12.221	16.510	14.960	1.00	3.97

FIG. 3AA

ATOM	1533	N	ILE	246	10.485	17.286	13.740	1.00	9.45
ATOM	1534	CA	ILE	246	10.551	16.235	12.724	1.00	9.45
ATOM	1535	CB	ILE	246	9.405	16.375	11.676	1.00	2.00
ATOM	1536	CG2	ILE	246	9.767	15.693	10.375	1.00	2.00
ATOM	1537	CG1	ILE	246	8.093	15.809	12.238	1.00	2.00
ATOM	1538	CD1	ILE	246	8.085	14.298	12.471	1.00	2.00
ATOM	1539	C	ILE	246	11.913	16.295	12.028	1.00	9.45
ATOM	1540	O	ILE	246	12.474	15.271	11.649	1.00	2.00
ATOM	1541	N	TRP	247	12.461	17.500	11.917	1.00	2.00
ATOM	1542	CA	TRP	247	13.753	17.696	11.297	1.00	2.00
ATOM	1543	CB	TRP	247	14.049	19.183	11.127	1.00	2.00
ATOM	1544	CG	TRP	247	15.459	19.469	10.711	1.00	2.00
ATOM	1545	CD2	TRP	247	15.952	19.627	9.377	1.00	2.00
ATOM	1546	CE2	TRP	247	17.341	19.837	9.466	1.00	2.00
ATOM	1547	CE3	TRP	247	15.352	19.599	8.116	1.00	2.00
ATOM	1548	CD1	TRP	247	16.547	19.600	11.530	1.00	2.00
ATOM	1549	NE1	TRP	247	17.678	19.820	10.793	1.00	2.00
ATOM	1550	CZ2	TRP	247	18.145	20.018	8.339	1.00	2.00
ATOM	1551	CZ3	TRP	247	16.147	19.779	6.998	1.00	2.00
ATOM	1552	CH2	TRP	247	17.528	19.982	7.113	1.00	2.00
ATOM	1553	C	TRP	247	14.830	17.070	12.161	1.00	2.00
ATOM	1554	O	TRP	247	15.710	16.386	11.659	1.00	2.00
ATOM	1555	N	SER	248	14.767	17.327	13.463	1.00	10.46
ATOM	1556	CA	SER	248	15.744	16.804	14.417	1.00	10.46
ATOM	1557	CB	SER	248	15.475	17.351	15.836	1.00	2.00
ATOM	1558	OG	SER	248	15.486	18.772	15.908	1.00	2.00
ATOM	1559	C	SER	248	15.677	15.271	14.411	1.00	10.46
ATOM	1560	O	SER	248	16.712	14.605	14.460	1.00	2.00
ATOM	1561	N	VAL	249	14.464	14.723	14.304	1.00	6.38
ATOM	1562	CA	VAL	249	14.250	13.275	14.267	1.00	6.38
ATOM	1563	CB	VAL	249	12.728	12.902	14.189	1.00	2.90
ATOM	1564	CG1	VAL	249	12.550	11.404	14.200	1.00	2.90
ATOM	1565	CG2	VAL	249	11.948	13.520	15.342	1.00	2.90
ATOM	1566	C	VAL	249	14.970	12.667	13.050	1.00	6.38
ATOM	1567	O	VAL	249	15.586	11.606	13.150	1.00	2.90
ATOM	1568	N	GLY	250	14.906	13.357	11.914	1.00	2.00
ATOM	1569	CA	GLY	250	15.545	12.883	10.698	1.00	2.00
ATOM	1570	C	GLY	250	17.060	12.971	10.710	1.00	2.00
ATOM	1571	O	GLY	250	17.732	12.207	10.021	1.00	20.96
ATOM	1572	N	CYS	251	17.600	13.908	11.482	1.00	11.18
ATOM	1573	CA	CYS	251	19.047	14.109	11.597	1.00	11.18
ATOM	1574	CB	CYS	251	19.359	15.372	12.409	1.00	6.78
ATOM	1575	SG	CYS	251	19.017	16.935	11.612	1.00	6.78
ATOM	1576	C	CYS	251	19.623	12.934	12.336	1.00	11.18
ATOM	1577	O	CYS	251	20.796	12.594	12.177	1.00	6.78
ATOM	1578	N	ILE	252	18.784	12.367	13.196	1.00	22.98
ATOM	1579	CA	ILE	252	19.134	11.218	14.005	1.00	22.98
ATOM	1580	CB	ILE	252	18.260	11.145	15.274	1.00	2.00
ATOM	1581	CG2	ILE	252	18.472	9.822	15.970	1.00	2.00
ATOM	1582	CG1	ILE	252	18.583	12.322	16.199	1.00	2.00
ATOM	1583	CD1	ILE	252	17.732	12.392	17.465	1.00	2.00
ATOM	1584	C	ILE	252	18.972	9.934	13.187	1.00	22.98
ATOM	1585	O	ILE	252	19.930	9.188	13.020	1.00	2.00
ATOM	1586	N	MET	253	17.783	9.704	12.634	1.00	2.00
ATOM	1587	CA	MET	253	17.538	8.505	11.849	1.00	2.00
ATOM	1588	CB	MET	253	16.152	8.544	11.217	1.00	4.75
ATOM	1589	CG	MET	253	15.880	7.401	10.253	1.00	4.75
ATOM	1590	SD	MET	253	14.288	7.565	9.443	1.00	4.75
ATOM	1591	CE	MET	253	14.189	6.019	8.680	1.00	4.75

FIG. 3BB

ATOM	1592	C	MET	253	18.582	8.364	10.758	1.00	2.00
ATOM	1593	O	MET	253	19.000	7.264	10.436	1.00	4.75
ATOM	1594	N	GLY	254	18.996	9.490	10.189	1.00	4.43
ATOM	1595	CA	GLY	254	19.992	9.481	9.136	1.00	4.43
ATOM	1596	C	GLY	254	21.359	9.089	9.655	1.00	4.43
ATOM	1597	O	GLY	254	22.172	8.552	8.915	1.00	19.89
ATOM	1598	N	GLU	255	21.605	9.360	10.933	1.00	26.96
ATOM	1599	CA	GLU	255	22.863	9.030	11.599	1.00	26.96
ATOM	1600	CB	GLU	255	23.051	9.943	12.817	1.00	19.79
ATOM	1601	CG	GLU	255	24.434	9.872	13.477	1.00	19.79
ATOM	1602	CD	GLU	255	24.713	11.057	14.392	1.00	19.79
ATOM	1603	OE1	GLU	255	23.824	11.922	14.531	1.00	19.79
ATOM	1604	OE2	GLU	255	25.821	11.136	14.952	1.00	19.79
ATOM	1605	C	GLU	255	22.872	7.551	12.017	1.00	26.96
ATOM	1606	O	GLU	255	23.920	6.903	11.997	1.00	19.79
ATOM	1607	N	MET	256	21.697	7.020	12.359	1.00	22.99
ATOM	1608	CA	MET	256	21.554	5.615	12.746	1.00	22.99
ATOM	1609	CB	MET	256	20.112	5.311	13.217	1.00	4.42
ATOM	1610	CG	MET	256	19.741	5.871	14.594	1.00	4.42
ATOM	1611	SD	MET	256	17.982	5.762	15.032	1.00	4.42
ATOM	1612	CE	MET	256	17.978	4.420	16.092	1.00	4.42
ATOM	1613	C	MET	256	21.873	4.754	11.514	1.00	22.99
ATOM	1614	O	MET	256	22.243	3.586	11.636	1.00	4.42
ATOM	1615	N	VAL	257	21.744	5.358	10.336	1.00	2.00
ATOM	1616	CA	VAL	257	21.982	4.700	9.057	1.00	2.00
ATOM	1617	CB	VAL	257	20.998	5.237	7.975	1.00	9.27
ATOM	1618	CG1	VAL	257	21.367	4.728	6.585	1.00	9.27
ATOM	1619	CG2	VAL	257	19.580	4.853	8.327	1.00	9.27
ATOM	1620	C	VAL	257	23.403	4.929	8.554	1.00	2.00
ATOM	1621	O	VAL	257	24.148	3.987	8.291	1.00	9.27
ATOM	1622	N	ARG	258	23.765	6.197	8.409	1.00	14.20
ATOM	1623	CA	ARG	258	25.076	6.575	7.907	1.00	14.20
ATOM	1624	CB	ARG	258	25.033	8.020	7.391	1.00	18.38
ATOM	1625	CG	ARG	258	25.598	8.182	6.001	1.00	18.38
ATOM	1626	CD	ARG	258	24.941	9.313	5.239	1.00	18.38
ATOM	1627	NE	ARG	258	25.581	10.606	5.471	1.00	18.38
ATOM	1628	CZ	ARG	258	25.359	11.703	4.740	1.00	18.38
ATOM	1629	NH1	ARG	258	24.515	11.676	3.714	1.00	18.38
ATOM	1630	NH2	ARG	258	25.963	12.844	5.055	1.00	18.38
ATOM	1631	C	ARG	258	26.196	6.398	8.926	1.00	14.20
ATOM	1632	O	ARG	258	27.369	6.369	8.566	1.00	18.38
ATOM	1633	N	HIS	259	25.828	6.243	10.195	1.00	6.43
ATOM	1634	CA	HIS	259	26.805	6.088	11.269	1.00	6.43
ATOM	1635	CB	HIS	259	27.510	4.740	11.163	1.00	14.61
ATOM	1636	CG	HIS	259	26.601	3.576	11.387	1.00	14.61
ATOM	1637	CD2	HIS	259	26.413	2.445	10.665	1.00	14.61
ATOM	1638	ND1	HIS	259	25.714	3.510	12.438	1.00	14.61
ATOM	1639	CE1	HIS	259	25.023	2.396	12.362	1.00	14.61
ATOM	1640	NE2	HIS	259	25.423	1.727	11.293	1.00	14.61
ATOM	1641	C	HIS	259	27.809	7.230	11.294	1.00	6.43
ATOM	1642	O	HIS	259	28.983	7.059	11.643	1.00	14.61
ATOM	1643	N	LYS	260	27.326	8.391	10.869	1.00	7.67
ATOM	1644	CA	LYS	260	28.085	9.627	10.848	1.00	7.67
ATOM	1645	CB	LYS	260	28.850	9.789	9.530	1.00	21.52
ATOM	1646	CG	LYS	260	30.252	9.148	9.536	1.00	21.52
ATOM	1647	CD	LYS	260	31.112	9.537	8.315	1.00	21.52
ATOM	1648	CE	LYS	260	30.605	8.933	7.012	1.00	21.52
ATOM	1649	NZ	LYS	260	31.486	9.290	5.853	1.00	21.52
ATOM	1650	C	LYS	260	27.043	10.723	11.024	1.00	7.67

FIG. 3CC

ATOM	1651	O	LYS	260	25.866	10.520	10.691	1.00	21.52
ATOM	1652	N	ILE	261	27.437	11.838	11.638	1.00	2.00
ATOM	1653	CA	ILE	261	26.515	12.950	11.844	1.00	2.00
ATOM	1654	CB	ILE	261	27.091	14.053	12.767	1.00	15.02
ATOM	1655	CG2	ILE	261	25.959	14.937	13.284	1.00	15.02
ATOM	1656	CG1	ILE	261	27.848	13.462	13.960	1.00	15.02
ATOM	1657	CD1	ILE	261	28.606	14.516	14.778	1.00	15.02
ATOM	1658	C	ILE	261	26.306	13.575	10.475	1.00	2.00
ATOM	1659	O	ILE	261	27.271	13.922	9.798	1.00	15.02
ATOM	1660	N	LEU	262	25.047	13.726	10.081	1.00	22.16
ATOM	1661	CA	LEU	262	24.700	14.298	8.777	1.00	22.16
ATOM	1662	CB	LEU	262	23.187	14.270	8.605	1.00	12.98
ATOM	1663	CG	LEU	262	22.463	12.931	8.609	1.00	12.98
ATOM	1664	CD1	LEU	262	21.008	13.190	8.267	1.00	12.98
ATOM	1665	CD2	LEU	262	23.091	12.011	7.588	1.00	12.98
ATOM	1666	C	LEU	262	25.237	15.724	8.471	1.00	22.16
ATOM	1667	O	LEU	262	25.986	15.922	7.498	1.00	12.98
ATOM	1668	N	PHE	263	24.841	16.707	9.280	1.00	2.00
ATOM	1669	CA	PHE	263	25.275	18.100	9.085	1.00	2.00
ATOM	1670	CB	PHE	263	24.065	19.009	8.802	1.00	7.82
ATOM	1671	CG	PHE	263	22.949	18.344	8.049	1.00	7.82
ATOM	1672	CD1	PHE	263	23.136	17.886	6.752	1.00	7.82
ATOM	1673	CD2	PHE	263	21.693	18.203	8.640	1.00	7.82
ATOM	1674	CE1	PHE	263	22.092	17.288	6.045	1.00	7.82
ATOM	1675	CE2	PHE	263	20.639	17.609	7.950	1.00	7.82
ATOM	1676	CZ	PHE	263	20.836	17.151	6.645	1.00	7.82
ATOM	1677	C	PHE	263	26.037	18.718	10.275	1.00	2.00
ATOM	1678	O	PHE	263	25.507	19.592	10.956	1.00	7.82
ATOM	1679	N	PRO	264	27.296	18.305	10.516	1.00	18.59
ATOM	1680	CD	PRO	264	28.074	17.296	9.787	1.00	14.60
ATOM	1681	CA	PRO	264	28.076	18.857	11.636	1.00	18.59
ATOM	1682	CB	PRO	264	29.412	18.102	11.540	1.00	14.60
ATOM	1683	CG	PRO	264	29.493	17.689	10.112	1.00	14.60
ATOM	1684	C	PRO	264	28.234	20.406	11.663	1.00	18.59
ATOM	1685	O	PRO	264	27.384	21.096	12.223	1.00	14.60
ATOM	1686	N	GLY	265	29.324	20.942	11.100	1.00	26.76
ATOM	1687	CA	GLY	265	29.525	22.387	11.085	1.00	26.76
ATOM	1688	C	GLY	265	29.901	23.014	12.425	1.00	26.76
ATOM	1689	O	GLY	265	29.130	22.947	13.381	1.00	2.00
ATOM	1690	N	ARG	266	31.090	23.622	12.487	1.00	2.58
ATOM	1691	CA	ARG	266	31.630	24.273	13.687	1.00	2.58
ATOM	1692	CB	ARG	266	32.986	24.918	13.394	1.00	31.96
ATOM	1693	CG	ARG	266	33.982	24.111	12.570	1.00	31.96
ATOM	1694	CD	ARG	266	34.966	25.050	11.846	1.00	31.96
ATOM	1695	NE	ARG	266	34.293	25.983	10.928	1.00	31.96
ATOM	1696	CZ	ARG	266	34.322	27.317	11.024	1.00	31.96
ATOM	1697	NH1	ARG	266	34.995	27.922	12.003	1.00	31.96
ATOM	1698	NH2	ARG	266	33.678	28.057	10.127	1.00	31.96
ATOM	1699	C	ARG	266	30.744	25.388	14.224	1.00	2.58
ATOM	1700	O	ARG	266	30.895	25.791	15.375	1.00	31.96
ATOM	1701	N	ASP	267	29.913	25.963	13.359	1.00	30.47
ATOM	1702	CA	ASP	267	29.020	27.052	13.754	1.00	30.47
ATOM	1703	CB	ASP	267	29.768	28.389	13.752	1.00	28.71
ATOM	1704	CG	ASP	267	30.417	28.705	12.404	1.00	28.71
ATOM	1705	OD1	ASP	267	31.125	27.838	11.841	1.00	28.71
ATOM	1706	OD2	ASP	267	30.237	29.841	11.909	1.00	28.71
ATOM	1707	C	ASP	267	27.827	27.121	12.814	1.00	30.47
ATOM	1708	O	ASP	267	27.903	26.623	11.688	1.00	28.71
ATOM	1709	N	TYR	268	26.761	27.799	13.253	1.00	13.24

FIG. 3DD

ATOM	1710	CA	TYR	268	25.538	27.933	12.455	1.00	13.24
ATOM	1711	CB	TYR	268	24.605	29.009	13.023	1.00	26.47
ATOM	1712	CG	TYR	268	23.570	28.524	14.025	1.00	26.47
ATOM	1713	CD1	TYR	268	23.432	27.170	14.343	1.00	26.47
ATOM	1714	CE1	TYR	268	22.499	26.737	15.321	1.00	26.47
ATOM	1715	CD2	TYR	268	22.750	29.432	14.692	1.00	26.47
ATOM	1716	CE2	TYR	268	21.820	29.012	15.663	1.00	26.47
ATOM	1717	CZ	TYR	268	21.700	27.668	15.978	1.00	26.47
ATOM	1718	OH	TYR	268	20.804	27.293	16.968	1.00	26.47
ATOM	1719	C	TYR	268	25.842	28.275	11.004	1.00	13.24
ATOM	1720	O	TYR	268	25.073	27.934	10.121	1.00	26.47
ATOM	1721	N	ILE	269	26.969	28.932	10.750	1.00	27.51
ATOM	1722	CA	ILE	269	27.340	29.299	9.383	1.00	27.51
ATOM	1723	CB	ILE	269	28.529	30.302	9.351	1.00	26.87
ATOM	1724	CG2	ILE	269	28.970	30.546	7.911	1.00	26.87
ATOM	1725	CG1	ILE	269	28.165	31.601	10.073	1.00	26.87
ATOM	1726	CD1	ILE	269	26.945	32.267	9.541	1.00	26.87
ATOM	1727	C	ILE	269	27.790	28.055	8.633	1.00	27.51
ATOM	1728	O	ILE	269	27.300	27.754	7.547	1.00	26.87
ATOM	1729	N	ASP	270	28.758	27.369	9.231	1.00	5.20
ATOM	1730	CA	ASP	270	29.347	26.161	8.692	1.00	5.20
ATOM	1731	CB	ASP	270	30.495	25.750	9.617	1.00	33.24
ATOM	1732	CG	ASP	270	31.302	24.588	9.078	1.00	33.24
ATOM	1733	OD1	ASP	270	31.141	24.228	7.891	1.00	33.24
ATOM	1734	OD2	ASP	270	32.119	24.025	9.838	1.00	33.24
ATOM	1735	C	ASP	270	28.304	25.045	8.624	1.00	5.20
ATOM	1736	O	ASP	270	28.338	24.183	7.746	1.00	33.24
ATOM	1737	N	GLN	271	27.351	25.093	9.543	1.00	25.51
ATOM	1738	CA	GLN	271	26.307	24.086	9.643	1.00	25.51
ATOM	1739	CB	GLN	271	25.621	24.244	10.990	1.00	9.91
ATOM	1740	CG	GLN	271	25.393	22.960	11.713	1.00	9.91
ATOM	1741	CD	GLN	271	23.953	22.572	11.694	1.00	9.91
ATOM	1742	OE1	GLN	271	23.133	23.178	12.380	1.00	9.91
ATOM	1743	NE2	GLN	271	23.623	21.567	10.904	1.00	9.91
ATOM	1744	C	GLN	271	25.290	24.156	8.515	1.00	25.51
ATOM	1745	O	GLN	271	24.834	23.130	8.025	1.00	9.91
ATOM	1746	N	TRP	272	24.920	25.371	8.129	1.00	2.00
ATOM	1747	CA	TRP	272	23.961	25.582	7.059	1.00	2.00
ATOM	1748	CB	TRP	272	23.501	27.034	7.055	1.00	2.00
ATOM	1749	CG	TRP	272	22.639	27.413	5.902	1.00	2.00
ATOM	1750	CD2	TRP	272	21.261	27.040	5.670	1.00	2.00
ATOM	1751	CE2	TRP	272	20.849	27.675	4.487	1.00	2.00
ATOM	1752	CE3	TRP	272	20.353	26.236	6.366	1.00	2.00
ATOM	1753	CD1	TRP	272	22.982	28.232	4.862	1.00	2.00
ATOM	1754	NE1	TRP	272	21.915	28.395	4.012	1.00	2.00
ATOM	1755	CZ2	TRP	272	19.550	27.524	3.966	1.00	2.00
ATOM	1756	CZ3	TRP	272	19.068	26.088	5.851	1.00	2.00
ATOM	1757	CH2	TRP	272	18.676	26.732	4.665	1.00	2.00
ATOM	1758	C	TRP	272	24.600	25.214	5.726	1.00	2.00
ATOM	1759	O	TRP	272	23.912	24.844	4.769	1.00	2.00
ATOM	1760	N	ASN	273	25.927	25.299	5.683	1.00	9.70
ATOM	1761	CA	ASN	273	26.686	24.971	4.489	1.00	9.70
ATOM	1762	CB	ASN	273	28.162	25.319	4.672	1.00	18.64
ATOM	1763	CG	ASN	273	28.395	26.809	4.841	1.00	18.64
ATOM	1764	OD1	ASN	273	29.434	27.219	5.338	1.00	18.64
ATOM	1765	ND2	ASN	273	27.430	27.627	4.423	1.00	18.64
ATOM	1766	C	ASN	273	26.532	23.493	4.208	1.00	9.70
ATOM	1767	O	ASN	273	26.176	23.100	3.098	1.00	18.64
ATOM	1768	N	LYS	274	26.704	22.685	5.247	1.00	3.97

FIG. 3EE

ATOM	1769	CA	LYS	274	26.578	21.239	5.140	1.00	3.97
ATOM	1770	CB	LYS	274	26.883	20.593	6.491	1.00	14.41
ATOM	1771	CG	LYS	274	28.160	21.077	7.123	1.00	14.41
ATOM	1772	CD	LYS	274	29.332	20.845	6.200	1.00	14.41
ATOM	1773	CE	LYS	274	29.818	19.414	6.283	1.00	14.41
ATOM	1774	NZ	LYS	274	30.453	19.182	7.591	1.00	14.41
ATOM	1775	C	LYS	274	25.167	20.838	4.701	1.00	3.97
ATOM	1776	O	LYS	274	25.002	19.940	3.880	1.00	14.41
ATOM	1777	N	VAL	275	24.161	21.537	5.224	1.00	11.35
ATOM	1778	CA	VAL	275	22.754	21.272	4.922	1.00	11.35
ATOM	1779	CB	VAL	275	21.819	22.227	5.715	1.00	13.06
ATOM	1780	CG1	VAL	275	20.365	22.029	5.313	1.00	13.06
ATOM	1781	CG2	VAL	275	21.993	21.993	7.191	1.00	13.06
ATOM	1782	C	VAL	275	22.410	21.417	3.446	1.00	11.35
ATOM	1783	O	VAL	275	21.724	20.569	2.877	1.00	13.06
ATOM	1784	N	ILE	276	22.852	22.523	2.851	1.00	34.01
ATOM	1785	CA	ILE	276	22.595	22.803	1.446	1.00	34.01
ATOM	1786	CB	ILE	276	22.666	24.326	1.152	1.00	6.67
ATOM	1787	CG2	ILE	276	21.498	25.023	1.810	1.00	6.67
ATOM	1788	CG1	ILE	276	24.022	24.894	1.595	1.00	6.67
ATOM	1789	CD1	ILE	276	24.279	26.346	1.194	1.00	6.67
ATOM	1790	C	ILE	276	23.550	22.040	0.529	1.00	34.01
ATOM	1791	O	ILE	276	23.224	21.748	-0.618	1.00	6.67
ATOM	1792	N	GLU	277	24.706	21.670	1.061	1.00	2.00
ATOM	1793	CA	GLU	277	25.694	20.930	0.302	1.00	2.00
ATOM	1794	CB	GLU	277	26.978	20.857	1.110	1.00	11.08
ATOM	1795	CG	GLU	277	28.227	20.945	0.298	1.00	11.08
ATOM	1796	CD	GLU	277	29.395	20.231	0.959	1.00	11.08
ATOM	1797	OE1	GLU	277	29.651	20.473	2.171	1.00	11.08
ATOM	1798	OE2	GLU	277	30.043	19.407	0.263	1.00	11.08
ATOM	1799	C	GLU	277	25.207	19.508	-0.002	1.00	2.00
ATOM	1800	O	GLU	277	25.833	18.784	-0.767	1.00	11.08
ATOM	1801	N	GLN	278	24.101	19.108	0.622	1.00	7.26
ATOM	1802	CA	GLN	278	23.533	17.775	0.450	1.00	7.26
ATOM	1803	CB	GLN	278	23.559	17.012	1.768	1.00	6.70
ATOM	1804	CG	GLN	278	24.939	16.832	2.353	1.00	6.70
ATOM	1805	CD	GLN	278	24.913	16.050	3.640	1.00	6.70
ATOM	1806	OE1	GLN	278	24.207	15.048	3.752	1.00	6.70
ATOM	1807	NE2	GLN	278	25.689	16.499	4.625	1.00	6.70
ATOM	1808	C	GLN	278	22.108	17.799	-0.054	1.00	7.26
ATOM	1809	O	GLN	278	21.830	17.340	-1.138	1.00	6.70
ATOM	1810	N	LEU	279	21.198	18.328	0.743	1.00	20.28
ATOM	1811	CA	LEU	279	19.796	18.364	0.352	1.00	20.28
ATOM	1812	CB	LEU	279	18.901	18.628	1.581	1.00	12.10
ATOM	1813	CG	LEU	279	19.274	18.001	2.944	1.00	12.10
ATOM	1814	CD1	LEU	279	18.256	18.392	3.985	1.00	12.10
ATOM	1815	CD2	LEU	279	19.386	16.480	2.881	1.00	12.10
ATOM	1816	C	LEU	279	19.550	19.393	-0.769	1.00	20.28
ATOM	1817	O	LEU	279	18.573	19.281	-1.511	1.00	12.10
ATOM	1818	N	GLY	280	20.467	20.354	-0.913	1.00	2.00
ATOM	1819	CA	GLY	280	20.350	21.385	-1.941	1.00	2.00
ATOM	1820	C	GLY	280	19.768	22.717	-1.489	1.00	2.00
ATOM	1821	O	GLY	280	19.066	22.779	-0.482	1.00	11.83
ATOM	1822	N	THR	281	20.046	23.787	-2.231	1.00	2.00
ATOM	1823	CA	THR	281	19.549	25.139	-1.917	1.00	2.00
ATOM	1824	CB	THR	281	20.145	26.205	-2.923	1.00	13.34
ATOM	1825	OG1	THR	281	21.582	26.144	-2.906	1.00	13.34
ATOM	1826	CG2	THR	281	19.701	27.628	-2.573	1.00	13.34
ATOM	1827	C	THR	281	17.999	25.181	-1.922	1.00	2.00

FIG. 3FF

ATOM	1828	O	THR	281	17.374	24.830	-2.920	1.00	13.34
ATOM	1829	N	PRO	282	17.375	25.631	-0.811	1.00	17.13
ATOM	1830	CD	PRO	282	17.997	26.220	0.386	1.00	3.54
ATOM	1831	CA	PRO	282	15.910	25.707	-0.698	1.00	17.13
ATOM	1832	CB	PRO	282	15.708	26.350	0.673	1.00	3.54
ATOM	1833	CG	PRO	282	16.915	27.164	0.859	1.00	3.54
ATOM	1834	C	PRO	282	15.172	26.484	-1.787	1.00	17.13
ATOM	1835	O	PRO	282	15.706	27.440	-2.357	1.00	3.54
ATOM	1836	N	CYS	283	13.934	26.072	-2.059	1.00	2.45
ATOM	1837	CA	CYS	283	13.110	26.728	-3.060	1.00	2.45
ATOM	1838	CB	CYS	283	11.796	25.953	-3.298	1.00	32.82
ATOM	1839	SG	CYS	283	10.506	26.042	-1.999	1.00	32.82
ATOM	1840	C	CYS	283	12.835	28.175	-2.664	1.00	2.45
ATOM	1841	O	CYS	283	12.799	28.512	-1.488	1.00	32.82
ATOM	1842	N	PRO	284	12.705	29.059	-3.658	1.00	29.31
ATOM	1843	CD	PRO	284	12.845	28.755	-5.094	1.00	30.81
ATOM	1844	CA	PRO	284	12.442	30.486	-3.464	1.00	29.31
ATOM	1845	CB	PRO	284	12.120	30.948	-4.885	1.00	30.81
ATOM	1846	CG	PRO	284	13.079	30.125	-5.696	1.00	30.81
ATOM	1847	C	PRO	284	11.324	30.801	-2.467	1.00	29.31
ATOM	1848	O	PRO	284	11.454	31.734	-1.667	1.00	30.81
ATOM	1849	N	ALA	285	10.251	30.008	-2.486	1.00	17.96
ATOM	1850	CA	ALA	285	9.144	30.230	-1.572	1.00	17.96
ATOM	1851	CB	ALA	285	8.084	29.158	-1.767	1.00	9.64
ATOM	1852	C	ALA	285	9.679	30.246	-0.124	1.00	17.96
ATOM	1853	O	ALA	285	9.308	31.119	0.660	1.00	9.64
ATOM	1854	N	PHE	286	10.630	29.358	0.176	1.00	4.52
ATOM	1855	CA	PHE	286	11.236	29.277	1.502	1.00	4.52
ATOM	1856	CB	PHE	286	12.185	28.079	1.578	1.00	4.64
ATOM	1857	CG	PHE	286	12.941	27.992	2.878	1.00	4.64
ATOM	1858	CD1	PHE	286	12.324	27.494	4.019	1.00	4.64
ATOM	1859	CD2	PHE	286	14.269	28.412	2.958	1.00	4.64
ATOM	1860	CE1	PHE	286	13.014	27.412	5.228	1.00	4.64
ATOM	1861	CE2	PHE	286	14.976	28.339	4.158	1.00	4.64
ATOM	1862	CZ	PHE	286	14.351	27.839	5.299	1.00	4.64
ATOM	1863	C	PHE	286	11.982	30.565	1.871	1.00	4.52
ATOM	1864	O	PHE	286	11.848	31.067	2.997	1.00	4.64
ATOM	1865	N	MET	287	12.748	31.100	0.915	1.00	19.98
ATOM	1866	CA	MET	287	13.511	32.333	1.097	1.00	19.98
ATOM	1867	CB	MET	287	14.371	32.602	-0.131	1.00	23.24
ATOM	1868	CG	MET	287	15.853	32.633	0.139	1.00	23.24
ATOM	1869	SD	MET	287	16.574	30.987	0.341	1.00	23.24
ATOM	1870	CE	MET	287	17.149	30.610	-1.343	1.00	23.24
ATOM	1871	C	MET	287	12.569	33.516	1.327	1.00	19.98
ATOM	1872	O	MET	287	12.876	34.423	2.114	1.00	23.24
ATOM	1873	N	LYS	288	11.419	33.493	0.657	1.00	9.91
ATOM	1874	CA	LYS	288	10.433	34.547	0.805	1.00	9.91
ATOM	1875	CB	LYS	288	9.204	34.256	-0.057	1.00	54.51
ATOM	1876	CG	LYS	288	9.363	34.698	-1.501	1.00	54.51
ATOM	1877	CD	LYS	288	8.116	34.431	-2.319	1.00	54.51
ATOM	1878	CE	LYS	288	8.376	34.747	-3.776	1.00	54.51
ATOM	1879	NZ	LYS	288	7.226	34.380	-4.654	1.00	54.51
ATOM	1880	C	LYS	288	10.021	34.703	2.259	1.00	9.91
ATOM	1881	O	LYS	288	9.599	35.778	2.680	1.00	54.51
ATOM	1882	N	LYS	289	10.180	33.631	3.028	1.00	48.86
ATOM	1883	CA	LYS	289	9.829	33.628	4.450	1.00	48.86
ATOM	1884	CB	LYS	289	9.502	32.196	4.896	1.00	28.25
ATOM	1885	CG	LYS	289	8.343	31.538	4.169	1.00	28.25
ATOM	1886	CD	LYS	289	8.255	30.064	4.554	1.00	28.25

FIG. 3GG

ATOM	1887	CE	LYS	289	6.927	29.444	4.131	1.00	28.25
ATOM	1888	NZ	LYS	289	6.843	28.016	4.540	1.00	28.25
ATOM	1889	C	LYS	289	10.949	34.195	5.351	1.00	48.86
ATOM	1890	O	LYS	289	10.723	34.521	6.519	1.00	28.25
ATOM	1891	N	LEU	290	12.143	34.336	4.791	1.00	16.09
ATOM	1892	CA	LEU	290	13.290	34.822	5.547	1.00	16.09
ATOM	1893	CB	LEU	290	14.585	34.379	4.870	1.00	23.78
ATOM	1894	CG	LEU	290	14.680	32.948	4.334	1.00	23.78
ATOM	1895	CD1	LEU	290	15.998	32.748	3.571	1.00	23.78
ATOM	1896	CD2	LEU	290	14.535	31.958	5.498	1.00	23.78
ATOM	1897	C	LEU	290	13.326	36.334	5.702	1.00	16.09
ATOM	1898	O	LEU	290	13.092	37.053	4.736	1.00	23.78
ATOM	1899	N	GLN	291	13.631	36.815	6.912	1.00	22.36
ATOM	1900	CA	GLN	291	13.741	38.257	7.177	1.00	22.36
ATOM	1901	CB	GLN	291	14.099	38.514	8.651	1.00	39.09
ATOM	1902	CG	GLN	291	14.582	39.946	8.993	1.00	39.09
ATOM	1903	CD	GLN	291	13.469	41.005	9.052	1.00	39.09
ATOM	1904	OE1	GLN	291	12.300	40.730	8.741	1.00	39.09
ATOM	1905	NE2	GLN	291	13.841	42.229	9.445	1.00	39.09
ATOM	1906	C	GLN	291	14.834	38.788	6.253	1.00	22.36
ATOM	1907	O	GLN	291	15.871	38.163	6.085	1.00	39.09
ATOM	1908	N	PRO	292	14.603	39.946	5.634	1.00	11.17
ATOM	1909	CD	PRO	292	13.414	40.780	5.878	1.00	16.09
ATOM	1910	CA	PRO	292	15.517	40.619	4.703	1.00	11.17
ATOM	1911	CB	PRO	292	15.015	42.058	4.739	1.00	16.09
ATOM	1912	CG	PRO	292	13.542	41.867	4.834	1.00	16.09
ATOM	1913	C	PRO	292	17.012	40.530	4.998	1.00	11.17
ATOM	1914	O	PRO	292	17.811	40.364	4.078	1.00	16.09
ATOM	1915	N	THR	293	17.393	40.618	6.266	1.00	4.79
ATOM	1916	CA	THR	293	18.810	40.573	6.611	1.00	4.79
ATOM	1917	CB	THR	293	19.140	41.301	7.945	1.00	13.45
ATOM	1918	OG1	THR	293	20.558	41.251	8.170	1.00	13.45
ATOM	1919	CG2	THR	293	18.408	40.668	9.117	1.00	13.45
ATOM	1920	C	THR	293	19.363	39.166	6.640	1.00	4.79
ATOM	1921	O	THR	293	20.577	38.978	6.577	1.00	13.45
ATOM	1922	N	VAL	294	18.467	38.190	6.770	1.00	44.45
ATOM	1923	CA	VAL	294	18.822	36.766	6.790	1.00	44.45
ATOM	1924	CB	VAL	294	17.930	35.976	7.779	1.00	21.86
ATOM	1925	CG1	VAL	294	18.343	34.522	7.801	1.00	21.86
ATOM	1926	CG2	VAL	294	18.022	36.592	9.172	1.00	21.86
ATOM	1927	C	VAL	294	18.624	36.181	5.383	1.00	44.45
ATOM	1928	O	VAL	294	19.312	35.224	4.984	1.00	21.86
ATOM	1929	N	ARG	295	17.686	36.779	4.642	1.00	2.00
ATOM	1930	CA	ARG	295	17.369	36.382	3.274	1.00	2.00
ATOM	1931	CB	ARG	295	16.106	37.102	2.794	1.00	35.93
ATOM	1932	CG	ARG	295	15.364	36.381	1.664	1.00	35.93
ATOM	1933	CD	ARG	295	14.280	37.240	1.010	1.00	35.93
ATOM	1934	NE	ARG	295	13.376	37.856	1.980	1.00	35.93
ATOM	1935	CZ	ARG	295	12.132	38.258	1.717	1.00	35.93
ATOM	1936	NH1	ARG	295	11.610	38.108	0.499	1.00	35.93
ATOM	1937	NH2	ARG	295	11.418	38.855	2.675	1.00	35.93
ATOM	1938	C	ARG	295	18.544	36.771	2.381	1.00	2.00
ATOM	1939	O	ARG	295	18.817	36.114	1.378	1.00	35.93
ATOM	1940	N	ASN	296	19.267	37.813	2.783	1.00	23.98
ATOM	1941	CA	ASN	296	20.415	38.294	2.031	1.00	23.98
ATOM	1942	CB	ASN	296	20.920	39.623	2.600	1.00	20.87
ATOM	1943	CG	ASN	296	21.628	40.454	1.560	1.00	20.87
ATOM	1944	OD1	ASN	296	20.986	41.240	0.865	1.00	20.87
ATOM	1945	ND2	ASN	296	22.929	40.219	1.371	1.00	20.87

FIG. 3HH

ATOM	1946	C	ASN	296	21.553	37.299	2.066	1.00	23.98
ATOM	1947	O	ASN	296	22.239	37.097	1.068	1.00	20.87
ATOM	1948	N	TYR	297	21.765	36.710	3.238	1.00	14.54
ATOM	1949	CA	TYR	297	22.823	35.738	3.463	1.00	14.54
ATOM	1950	CB	TYR	297	22.878	35.396	4.955	1.00	12.06
ATOM	1951	CG	TYR	297	23.853	34.309	5.295	1.00	12.06
ATOM	1952	CD1	TYR	297	25.221	34.513	5.171	1.00	12.06
ATOM	1953	CE1	TYR	297	26.133	33.509	5.481	1.00	12.06
ATOM	1954	CD2	TYR	297	23.411	33.070	5.739	1.00	12.06
ATOM	1955	CE2	TYR	297	24.318	32.056	6.050	1.00	12.06
ATOM	1956	CZ	TYR	297	25.678	32.284	5.918	1.00	12.06
ATOM	1957	OH	TYR	297	26.579	31.288	6.223	1.00	12.06
ATOM	1958	C	TYR	297	22.646	34.464	2.648	1.00	14.54
ATOM	1959	O	TYR	297	23.561	34.036	1.941	1.00	12.06
ATOM	1960	N	VAL	298	21.449	33.892	2.747	1.00	4.63
ATOM	1961	CA	VAL	298	21.088	32.656	2.077	1.00	4.63
ATOM	1962	CB	VAL	298	19.723	32.124	2.581	1.00	42.51
ATOM	1963	CG1	VAL	298	19.304	30.882	1.785	1.00	42.51
ATOM	1964	CG2	VAL	298	19.790	31.802	4.064	1.00	42.51
ATOM	1965	C	VAL	298	21.010	32.784	0.565	1.00	4.63
ATOM	1966	O	VAL	298	21.485	31.898	-0.163	1.00	42.51
ATOM	1967	N	GLU	299	20.388	33.859	0.080	1.00	21.61
ATOM	1968	CA	GLU	299	20.264	34.064	-1.361	1.00	21.61
ATOM	1969	CB	GLU	299	19.329	35.220	-1.671	1.00	40.37
ATOM	1970	CG	GLU	299	17.884	34.920	-1.312	1.00	40.37
ATOM	1971	CD	GLU	299	16.986	36.142	-1.378	1.00	40.37
ATOM	1972	OE1	GLU	299	17.464	37.260	-1.076	1.00	40.37
ATOM	1973	OE2	GLU	299	15.802	35.984	-1.722	1.00	40.37
ATOM	1974	C	GLU	299	21.632	34.301	-1.973	1.00	21.61
ATOM	1975	O	GLU	299	21.957	33.735	-3.015	1.00	40.37
ATOM	1976	N	ASN	300	22.455	35.104	-1.310	1.00	5.94
ATOM	1977	CA	ASN	300	23.790	35.372	-1.818	1.00	5.94
ATOM	1978	CB	ASN	300	24.185	36.816	-1.512	1.00	39.13
ATOM	1979	CG	ASN	300	23.274	37.827	-2.201	1.00	39.13
ATOM	1980	OD1	ASN	300	23.558	38.274	-3.314	1.00	39.13
ATOM	1981	ND2	ASN	300	22.163	38.168	-1.558	1.00	39.13
ATOM	1982	C	ASN	300	24.743	34.356	-1.193	1.00	5.94
ATOM	1983	O	ASN	300	25.658	34.706	-0.441	1.00	39.13
ATOM	1984	N	ARG	301	24.494	33.087	-1.505	1.00	26.43
ATOM	1985	CA	ARG	301	25.280	31.956	-1.005	1.00	26.43
ATOM	1986	CB	ARG	301	24.505	31.286	0.153	1.00	45.38
ATOM	1987	CG	ARG	301	25.323	30.477	1.138	1.00	45.38
ATOM	1988	CD	ARG	301	25.484	31.225	2.445	1.00	45.38
ATOM	1989	NE	ARG	301	26.760	30.897	3.071	1.00	45.38
ATOM	1990	CZ	ARG	301	27.869	31.633	2.959	1.00	45.38
ATOM	1991	NH1	ARG	301	27.870	32.759	2.249	1.00	45.38
ATOM	1992	NH2	ARG	301	29.001	31.208	3.510	1.00	45.38
ATOM	1993	C	ARG	301	25.469	30.955	-2.158	1.00	26.43
ATOM	1994	O	ARG	301	24.525	30.686	-2.903	1.00	45.38
ATOM	1995	N	PRO	302	26.684	30.392	-2.315	1.00	7.81
ATOM	1996	CD	PRO	302	27.840	30.490	-1.414	1.00	9.65
ATOM	1997	CA	PRO	302	26.953	29.424	-3.387	1.00	7.81
ATOM	1998	CB	PRO	302	28.326	28.860	-3.009	1.00	9.65
ATOM	1999	CG	PRO	302	28.420	29.106	-1.534	1.00	9.65
ATOM	2000	C	PRO	302	25.885	28.348	-3.432	1.00	7.81
ATOM	2001	O	PRO	302	25.600	27.715	-2.419	1.00	9.65
ATOM	2002	N	LYS	303	25.279	28.166	-4.604	1.00	38.56
ATOM	2003	CA	LYS	303	24.195	27.191	-4.785	1.00	38.56
ATOM	2004	CB	LYS	303	23.260	27.627	-5.923	1.00	37.34

FIG. 3II

ATOM	2005	CG	LYS	303	22.529	28.920	-5.637	1.00	37.34
ATOM	2006	CD	LYS	303	21.645	29.313	-6.794	1.00	37.34
ATOM	2007	CE	LYS	303	21.230	30.779	-6.697	1.00	37.34
ATOM	2008	NZ	LYS	303	20.640	31.268	-7.995	1.00	37.34
ATOM	2009	C	LYS	303	24.587	25.738	-4.989	1.00	38.56
ATOM	2010	O	LYS	303	25.719	25.429	-5.367	1.00	37.34
ATOM	2011	N	TYR	304	23.626	24.859	-4.692	1.00	20.93
ATOM	2012	CA	TYR	304	23.768	23.405	-4.834	1.00	20.93
ATOM	2013	CB	TYR	304	24.093	22.741	-3.501	1.00	13.21
ATOM	2014	CG	TYR	304	25.503	22.977	-3.082	1.00	13.21
ATOM	2015	CD1	TYR	304	26.536	22.201	-3.585	1.00	13.21
ATOM	2016	CE1	TYR	304	27.853	22.469	-3.252	1.00	13.21
ATOM	2017	CD2	TYR	304	25.814	24.013	-2.219	1.00	13.21
ATOM	2018	CE2	TYR	304	27.120	24.291	-1.876	1.00	13.21
ATOM	2019	CZ	TYR	304	28.141	23.522	-2.391	1.00	13.21
ATOM	2020	OH	TYR	304	29.441	23.858	-2.075	1.00	13.21
ATOM	2021	C	TYR	304	22.492	22.796	-5.388	1.00	20.93
ATOM	2022	O	TYR	304	21.395	23.037	-4.878	1.00	13.21
ATOM	2023	N	ALA	305	22.645	22.006	-6.446	1.00	21.50
ATOM	2024	CA	ALA	305	21.513	21.354	-7.096	1.00	21.50
ATOM	2025	CB	ALA	305	21.991	20.549	-8.290	1.00	20.54
ATOM	2026	C	ALA	305	20.815	20.454	-6.102	1.00	21.50
ATOM	2027	O	ALA	305	19.593	20.350	-6.103	1.00	20.54
ATOM	2028	N	GLY	306	21.613	19.836	-5.230	1.00	20.44
ATOM	2029	CA	GLY	306	21.093	18.937	-4.213	1.00	20.44
ATOM	2030	C	GLY	306	21.169	17.482	-4.628	1.00	20.44
ATOM	2031	O	GLY	306	20.868	17.134	-5.778	1.00	20.50
ATOM	2032	N	LEU	307	21.615	16.640	-3.703	1.00	6.20
ATOM	2033	CA	LEU	307	21.729	15.209	-3.939	1.00	6.20
ATOM	2034	CB	LEU	307	22.836	14.598	-3.085	1.00	18.44
ATOM	2035	CG	LEU	307	24.157	15.349	-2.934	1.00	18.44
ATOM	2036	CD1	LEU	307	25.127	14.529	-2.083	1.00	18.44
ATOM	2037	CD2	LEU	307	24.744	15.651	-4.303	1.00	18.44
ATOM	2038	C	LEU	307	20.413	14.550	-3.562	1.00	6.20
ATOM	2039	O	LEU	307	19.789	14.910	-2.561	1.00	18.44
ATOM	2040	N	THR	308	19.993	13.589	-4.379	1.00	50.96
ATOM	2041	CA	THR	308	18.753	12.861	-4.133	1.00	50.96
ATOM	2042	CB	THR	308	18.299	12.053	-5.389	1.00	9.59
ATOM	2043	OG1	THR	308	19.303	11.094	-5.751	1.00	9.59
ATOM	2044	CG2	THR	308	18.040	12.992	-6.557	1.00	9.59
ATOM	2045	C	THR	308	18.953	11.929	-2.928	1.00	50.96
ATOM	2046	O	THR	308	20.082	11.559	-2.596	1.00	9.59
ATOM	2047	N	PHE	309	17.856	11.538	-2.289	1.00	9.28
ATOM	2048	CA	PHE	309	17.953	10.679	-1.123	1.00	9.28
ATOM	2049	CB	PHE	309	16.612	10.561	-0.421	1.00	35.97
ATOM	2050	CG	PHE	309	16.280	11.795	0.378	1.00	35.97
ATOM	2051	CD1	PHE	309	16.772	11.950	1.675	1.00	35.97
ATOM	2052	CD2	PHE	309	15.577	12.854	-0.203	1.00	35.97
ATOM	2053	CE1	PHE	309	16.575	13.149	2.387	1.00	35.97
ATOM	2054	CE2	PHE	309	15.373	14.062	0.497	1.00	35.97
ATOM	2055	CZ	PHE	309	15.875	14.205	1.796	1.00	35.97
ATOM	2056	C	PHE	309	18.637	9.355	-1.354	1.00	9.28
ATOM	2057	O	PHE	309	19.450	8.940	-0.542	1.00	35.97
ATOM	2058	N	PRO	310	18.371	8.699	-2.495	1.00	38.48
ATOM	2059	CD	PRO	310	17.483	8.981	-3.638	1.00	23.38
ATOM	2060	CA	PRO	310	19.075	7.426	-2.677	1.00	38.48
ATOM	2061	CB	PRO	310	18.467	6.875	-3.970	1.00	23.38
ATOM	2062	CG	PRO	310	18.106	8.120	-4.738	1.00	23.38
ATOM	2063	C	PRO	310	20.584	7.675	-2.794	1.00	38.48

FIG. 3JJ

ATOM	2064	O	PRO	310	21.373	6.834	-2.378	1.00	23.38
ATOM	2065	N	LYS	311	20.971	8.846	-3.308	1.00	13.04
ATOM	2066	CA	LYS	311	22.385	9.214	-3.465	1.00	13.04
ATOM	2067	CB	LYS	311	22.523	10.463	-4.342	1.00	34.06
ATOM	2068	CG	LYS	311	22.808	10.195	-5.807	1.00	34.06
ATOM	2069	CD	LYS	311	24.240	9.693	-6.011	1.00	34.06
ATOM	2070	CE	LYS	311	24.521	9.395	-7.494	1.00	34.06
ATOM	2071	NZ	LYS	311	25.967	9.063	-7.743	1.00	34.06
ATOM	2072	C	LYS	311	23.019	9.494	-2.105	1.00	13.04
ATOM	2073	O	LYS	311	24.187	9.171	-1.865	1.00	34.06
ATOM	2074	N	LEU	312	22.234	10.137	-1.241	1.00	30.77
ATOM	2075	CA	LEU	312	22.635	10.500	0.118	1.00	30.77
ATOM	2076	CB	LEU	312	21.673	11.556	0.665	1.00	12.53
ATOM	2077	CG	LEU	312	21.900	13.005	0.240	1.00	12.53
ATOM	2078	CD1	LEU	312	20.660	13.854	0.540	1.00	12.53
ATOM	2079	CD2	LEU	312	23.134	13.523	0.958	1.00	12.53
ATOM	2080	C	LEU	312	22.658	9.285	1.060	1.00	30.77
ATOM	2081	O	LEU	312	23.514	9.193	1.953	1.00	12.53
ATOM	2082	N	PHE	313	21.709	8.376	0.860	1.00	9.82
ATOM	2083	CA	PHE	313	21.600	7.167	1.668	1.00	9.82
ATOM	2084	CB	PHE	313	20.302	7.155	2.486	1.00	19.45
ATOM	2085	CG	PHE	313	20.168	8.307	3.440	1.00	19.45
ATOM	2086	CD1	PHE	313	21.030	8.435	4.522	1.00	19.45
ATOM	2087	CD2	PHE	313	19.182	9.268	3.235	1.00	19.45
ATOM	2088	CE1	PHE	313	20.930	9.493	5.385	1.00	19.45
ATOM	2089	CE2	PHE	313	19.056	10.349	4.085	1.00	19.45
ATOM	2090	CZ	PHE	313	19.938	10.468	5.172	1.00	19.45
ATOM	2091	C	PHE	313	21.559	5.977	0.718	1.00	9.82
ATOM	2092	O	PHE	313	20.501	5.371	0.525	1.00	19.45
ATOM	2093	N	PRO	314	22.709	5.608	0.128	1.00	17.77
ATOM	2094	CD	PRO	314	24.077	6.031	0.454	1.00	21.65
ATOM	2095	CA	PRO	314	22.726	4.474	-0.797	1.00	17.77
ATOM	2096	CB	PRO	314	24.203	4.367	-1.168	1.00	21.65
ATOM	2097	CG	PRO	314	24.881	4.791	0.098	1.00	21.65
ATOM	2098	C	PRO	314	22.227	3.213	-0.114	1.00	17.77
ATOM	2099	O	PRO	314	22.160	3.142	1.111	1.00	21.65
ATOM	2100	N	ASP	315	21.889	2.215	-0.919	1.00	38.72
ATOM	2101	CA	ASP	315	21.380	0.941	-0.422	1.00	38.72
ATOM	2102	CB	ASP	315	21.078	0.026	-1.610	1.00	47.92
ATOM	2103	CG	ASP	315	20.157	0.687	-2.626	1.00	47.92
ATOM	2104	OD1	ASP	315	18.939	0.386	-2.604	1.00	47.92
ATOM	2105	OD2	ASP	315	20.646	1.517	-3.434	1.00	47.92
ATOM	2106	C	ASP	315	22.324	0.248	0.568	1.00	38.72
ATOM	2107	O	ASP	315	21.888	-0.275	1.600	1.00	47.92
ATOM	2108	N	SER	316	23.623	0.348	0.301	1.00	22.14
ATOM	2109	CA	SER	316	24.645	-0.274	1.130	1.00	22.14
ATOM	2110	CB	SER	316	26.022	0.086	0.593	1.00	41.15
ATOM	2111	OG	SER	316	26.118	1.482	0.360	1.00	41.15
ATOM	2112	C	SER	316	24.587	0.026	2.622	1.00	22.14
ATOM	2113	O	SER	316	25.207	-0.678	3.411	1.00	41.15
ATOM	2114	N	LEU	317	23.846	1.057	3.014	1.00	35.08
ATOM	2115	CA	LEU	317	23.741	1.414	4.427	1.00	35.08
ATOM	2116	CB	LEU	317	23.445	2.903	4.586	1.00	17.46
ATOM	2117	CG	LEU	317	24.520	3.820	4.021	1.00	17.46
ATOM	2118	CD1	LEU	317	24.047	5.257	4.043	1.00	17.46
ATOM	2119	CD2	LEU	317	25.812	3.628	4.797	1.00	17.46
ATOM	2120	C	LEU	317	22.659	0.599	5.118	1.00	35.08
ATOM	2121	O	LEU	317	22.862	0.095	6.229	1.00	17.46
ATOM	2122	N	PHE	318	21.531	0.455	4.435	1.00	4.02

FIG. 3KK

ATOM	2123	CA	PHE	318	20.392	-0.278	4.954	1.00	4.02
ATOM	2124	CB	PHE	318	19.113	0.147	4.230	1.00	16.56
ATOM	2125	CG	PHE	318	18.903	1.640	4.201	1.00	16.56
ATOM	2126	CD1	PHE	318	18.133	2.268	5.174	1.00	16.56
ATOM	2127	CD2	PHE	318	19.514	2.420	3.216	1.00	16.56
ATOM	2128	CE1	PHE	318	17.977	3.655	5.175	1.00	16.56
ATOM	2129	CE2	PHE	318	19.373	3.805	3.201	1.00	16.56
ATOM	2130	CZ	PHE	318	18.602	4.430	4.182	1.00	16.56
ATOM	2131	C	PHE	318	20.591	-1.758	4.744	1.00	4.02
ATOM	2132	O	PHE	318	21.200	-2.172	3.761	1.00	16.56
ATOM	2133	N	PRO	319	20.151	-2.578	5.708	1.00	31.17
ATOM	2134	CD	PRO	319	19.637	-2.218	7.040	1.00	52.46
ATOM	2135	CA	PRO	319	20.289	-4.029	5.574	1.00	31.17
ATOM	2136	CB	PRO	319	19.834	-4.543	6.951	1.00	52.46
ATOM	2137	CG	PRO	319	18.905	-3.478	7.455	1.00	52.46
ATOM	2138	C	PRO	319	19.339	-4.452	4.451	1.00	31.17
ATOM	2139	O	PRO	319	18.128	-4.225	4.536	1.00	52.46
ATOM	2140	N	ALA	320	19.881	-5.025	3.384	1.00	10.87
ATOM	2141	CA	ALA	320	19.059	-5.424	2.257	1.00	10.87
ATOM	2142	CB	ALA	320	19.248	-4.435	1.107	1.00	25.21
ATOM	2143	C	ALA	320	19.414	-6.826	1.808	1.00	10.87
ATOM	2144	O	ALA	320	19.881	-7.020	0.685	1.00	25.21
ATOM	2145	N	ASP	321	19.203	-7.804	2.685	1.00	47.66
ATOM	2146	CA	ASP	321	19.521	-9.181	2.338	1.00	47.66
ATOM	2147	CB	ASP	321	20.236	-9.900	3.483	1.00	64.42
ATOM	2148	CG	ASP	321	21.094	-11.050	2.986	1.00	64.42
ATOM	2149	OD1	ASP	321	21.230	-11.200	1.744	1.00	64.42
ATOM	2150	OD2	ASP	321	21.630	-11.811	3.820	1.00	64.42
ATOM	2151	C	ASP	321	18.294	-9.956	1.891	1.00	47.66
ATOM	2152	O	ASP	321	18.337	-10.675	0.893	1.00	64.42
ATOM	2153	N	SER	322	17.222	-9.840	2.661	1.00	3.49
ATOM	2154	CA	SER	322	15.970	-10.494	2.337	1.00	3.49
ATOM	2155	CB	SER	322	15.264	-10.922	3.612	1.00	13.00
ATOM	2156	OG	SER	322	15.170	-9.836	4.520	1.00	13.00
ATOM	2157	C	SER	322	15.094	-9.500	1.589	1.00	3.49
ATOM	2158	O	SER	322	15.394	-8.315	1.528	1.00	13.00
ATOM	2159	N	GLU	323	13.978	-9.983	1.070	1.00	2.00
ATOM	2160	CA	GLU	323	13.051	-9.146	0.331	1.00	2.00
ATOM	2161	CB	GLU	323	12.168	-10.007	-0.567	1.00	23.86
ATOM	2162	CG	GLU	323	11.838	-9.356	-1.886	1.00	23.86
ATOM	2163	CD	GLU	323	12.668	-9.902	-3.036	1.00	23.86
ATOM	2164	OE1	GLU	323	12.195	-10.834	-3.713	1.00	23.86
ATOM	2165	OE2	GLU	323	13.781	-9.396	-3.284	1.00	23.86
ATOM	2166	C	GLU	323	12.194	-8.306	1.276	1.00	2.00
ATOM	2167	O	GLU	323	11.431	-7.448	0.837	1.00	23.86
ATOM	2168	N	HIS	324	12.283	-8.598	2.570	1.00	17.95
ATOM	2169	CA	HIS	324	11.560	-7.852	3.605	1.00	17.95
ATOM	2170	CB	HIS	324	11.312	-8.750	4.834	1.00	5.49
ATOM	2171	CG	HIS	324	10.841	-8.010	6.060	1.00	5.49
ATOM	2172	CD2	HIS	324	9.611	-7.862	6.596	1.00	5.49
ATOM	2173	ND1	HIS	324	11.713	-7.370	6.917	1.00	5.49
ATOM	2174	CE1	HIS	324	11.036	-6.861	7.928	1.00	5.49
ATOM	2175	NE2	HIS	324	9.759	-7.144	7.763	1.00	5.49
ATOM	2176	C	HIS	324	12.466	-6.686	3.969	1.00	17.95
ATOM	2177	O	HIS	324	12.003	-5.582	4.224	1.00	5.49
ATOM	2178	N	ASN	325	13.767	-6.953	3.993	1.00	2.00
ATOM	2179	CA	ASN	325	14.774	-5.943	4.293	1.00	2.00
ATOM	2180	CB	ASN	325	16.103	-6.609	4.656	1.00	16.84

FIG. 3LL

ATOM	2181	CG	ASN	325	16.090	-7.208	6.039	1.00	16.84
ATOM	2182	OD1	ASN	325	15.032	-7.379	6.645	1.00	16.84
ATOM	2183	ND2	ASN	325	17.263	-7.517	6.558	1.00	16.84
ATOM	2184	C	ASN	325	14.984	-5.004	3.122	1.00	2.00
ATOM	2185	O	ASN	325	15.645	-3.982	3.246	1.00	16.84
ATOM	2186	N	LYS	326	14.468	-5.386	1.964	1.00	23.08
ATOM	2187	CA	LYS	326	14.582	-4.552	0.791	1.00	23.08
ATOM	2188	CB	LYS	326	14.644	-5.405	-0.475	1.00	28.36
ATOM	2189	CG	LYS	326	15.917	-6.240	-0.575	1.00	28.36
ATOM	2190	CD	LYS	326	15.960	-6.997	-1.888	1.00	28.36
ATOM	2191	CE	LYS	326	17.085	-8.035	-1.946	1.00	28.36
ATOM	2192	NZ	LYS	326	18.456	-7.449	-2.017	1.00	28.36
ATOM	2193	C	LYS	326	13.387	-3.608	0.766	1.00	23.08
ATOM	2194	O	LYS	326	13.531	-2.426	0.465	1.00	28.36
ATOM	2195	N	LEU	327	12.220	-4.107	1.150	1.00	2.00
ATOM	2196	CA	LEU	327	11.028	-3.277	1.165	1.00	2.00
ATOM	2197	CB	LEU	327	9.772	-4.119	1.385	1.00	8.67
ATOM	2198	CG	LEU	327	8.421	-3.402	1.491	1.00	8.67
ATOM	2199	CD1	LEU	327	8.096	-2.695	0.196	1.00	8.67
ATOM	2200	CD2	LEU	327	7.319	-4.379	1.836	1.00	8.67
ATOM	2201	C	LEU	327	11.150	-2.229	2.249	1.00	2.00
ATOM	2202	O	LEU	327	10.984	-1.047	1.993	1.00	8.67
ATOM	2203	N	LYS	328	11.489	-2.656	3.452	1.00	2.57
ATOM	2204	CA	LYS	328	11.634	-1.739	4.570	1.00	2.57
ATOM	2205	CB	LYS	328	11.946	-2.510	5.852	1.00	9.10
ATOM	2206	CG	LYS	328	10.761	-3.238	6.441	1.00	9.10
ATOM	2207	CD	LYS	328	9.688	-2.273	6.894	1.00	9.10
ATOM	2208	CE	LYS	328	8.459	-3.009	7.391	1.00	9.10
ATOM	2209	NZ	LYS	328	7.431	-2.129	8.011	1.00	9.10
ATOM	2210	C	LYS	328	12.703	-0.680	4.324	1.00	2.57
ATOM	2211	O	LYS	328	12.585	0.441	4.802	1.00	9.10
ATOM	2212	N	ALA	329	13.716	-1.029	3.541	1.00	13.58
ATOM	2213	CA	ALA	329	14.804	-0.117	3.230	1.00	13.58
ATOM	2214	CB	ALA	329	15.970	-0.865	2.596	1.00	16.18
ATOM	2215	C	ALA	329	14.337	0.997	2.317	1.00	13.58
ATOM	2216	O	ALA	329	14.899	2.079	2.341	1.00	16.18
ATOM	2217	N	SER	330	13.330	0.726	1.491	1.00	11.09
ATOM	2218	CA	SER	330	12.785	1.737	0.593	1.00	11.09
ATOM	2219	CB	SER	330	12.081	1.100	-0.611	1.00	11.72
ATOM	2220	OG	SER	330	10.754	0.706	-0.292	1.00	11.72
ATOM	2221	C	SER	330	11.806	2.581	1.404	1.00	11.09
ATOM	2222	O	SER	330	11.557	3.743	1.093	1.00	11.72
ATOM	2223	N	GLN	331	11.266	1.986	2.461	1.00	2.00
ATOM	2224	CA	GLN	331	10.333	2.679	3.335	1.00	2.00
ATOM	2225	CB	GLN	331	9.517	1.664	4.131	1.00	6.13
ATOM	2226	CG	GLN	331	8.571	0.855	3.293	1.00	6.13
ATOM	2227	CD	GLN	331	7.766	-0.121	4.097	1.00	6.13
ATOM	2228	OE1	GLN	331	8.024	-0.337	5.265	1.00	6.13
ATOM	2229	NE2	GLN	331	6.795	-0.740	3.463	1.00	6.13
ATOM	2230	C	GLN	331	11.058	3.617	4.298	1.00	2.00
ATOM	2231	O	GLN	331	10.513	4.639	4.717	1.00	6.13
ATOM	2232	N	ALA	332	12.277	3.235	4.660	1.00	5.63
ATOM	2233	CA	ALA	332	13.102	3.992	5.583	1.00	5.63
ATOM	2234	CB	ALA	332	14.277	3.151	6.043	1.00	19.90
ATOM	2235	C	ALA	332	13.603	5.241	4.909	1.00	5.63
ATOM	2236	O	ALA	332	13.528	6.333	5.459	1.00	19.90
ATOM	2237	N	ARG	333	14.053	5.080	3.676	1.00	2.00
ATOM	2238	CA	ARG	333	14.575	6.186	2.902	1.00	2.00

FIG. 3MM

ATOM	2239	CB	ARG	333	15.351	5.665	1.703	1.00	16.50
ATOM	2240	CG	ARG	333	16.331	6.648	1.131	1.00	16.50
ATOM	2241	CD	ARG	333	16.800	6.190	-0.246	1.00	16.50
ATOM	2242	NE	ARG	333	17.762	5.090	-0.231	1.00	16.50
ATOM	2243	CZ	ARG	333	17.581	3.920	-0.842	1.00	16.50
ATOM	2244	NH1	ARG	333	16.452	3.680	-1.502	1.00	16.50
ATOM	2245	NH2	ARG	333	18.572	3.028	-0.877	1.00	16.50
ATOM	2246	C	ARG	333	13.442	7.095	2.461	1.00	2.00
ATOM	2247	O	ARG	333	13.655	8.281	2.266	1.00	16.50
ATOM	2248	N	ASP	334	12.229	6.561	2.349	1.00	2.00
ATOM	2249	CA	ASP	334	11.095	7.377	1.953	1.00	2.00
ATOM	2250	CB	ASP	334	9.887	6.522	1.588	1.00	11.10
ATOM	2251	CG	ASP	334	8.753	7.341	0.973	1.00	11.10
ATOM	2252	OD1	ASP	334	8.940	7.907	-0.137	1.00	11.10
ATOM	2253	OD2	ASP	334	7.670	7.412	1.594	1.00	11.10
ATOM	2254	C	ASP	334	10.712	8.286	3.110	1.00	2.00
ATOM	2255	O	ASP	334	10.309	9.425	2.904	1.00	11.10
ATOM	2256	N	LEU	335	10.803	7.756	4.325	1.00	2.00
ATOM	2257	CA	LEU	335	10.486	8.491	5.536	1.00	2.00
ATOM	2258	CB	LEU	335	10.486	7.523	6.717	1.00	2.00
ATOM	2259	CG	LEU	335	10.094	7.963	8.118	1.00	2.00
ATOM	2260	CD1	LEU	335	8.660	8.436	8.151	1.00	2.00
ATOM	2261	CD2	LEU	335	10.295	6.800	9.052	1.00	2.00
ATOM	2262	C	LEU	335	11.555	9.561	5.700	1.00	2.00
ATOM	2263	O	LEU	335	11.239	10.719	5.931	1.00	2.00
ATOM	2264	N	LEU	336	12.814	9.181	5.511	1.00	2.14
ATOM	2265	CA	LEU	336	13.925	10.111	5.611	1.00	2.14
ATOM	2266	CB	LEU	336	15.250	9.392	5.335	1.00	8.04
ATOM	2267	CG	LEU	336	16.116	8.862	6.472	1.00	8.04
ATOM	2268	CD1	LEU	336	17.147	7.889	5.941	1.00	8.04
ATOM	2269	CD2	LEU	336	16.786	10.022	7.172	1.00	8.04
ATOM	2270	C	LEU	336	13.775	11.280	4.625	1.00	2.14
ATOM	2271	O	LEU	336	14.096	12.423	4.968	1.00	8.04
ATOM	2272	N	SER	337	13.277	10.995	3.419	1.00	2.00
ATOM	2273	CA	SER	337	13.098	12.009	2.386	1.00	2.00
ATOM	2274	CB	SER	337	12.788	11.367	1.024	1.00	2.98
ATOM	2275	OG	SER	337	11.543	10.693	1.022	1.00	2.98
ATOM	2276	C	SER	337	12.022	13.024	2.722	1.00	2.00
ATOM	2277	O	SER	337	11.999	14.103	2.151	1.00	2.98
ATOM	2278	N	LYS	338	11.110	12.658	3.616	1.00	3.30
ATOM	2279	CA	LYS	338	10.031	13.539	4.030	1.00	3.30
ATOM	2280	CB	LYS	338	8.796	12.733	4.438	1.00	10.86
ATOM	2281	CG	LYS	338	8.340	11.631	3.484	1.00	10.86
ATOM	2282	CD	LYS	338	7.473	12.142	2.349	1.00	10.86
ATOM	2283	CE	LYS	338	6.938	10.996	1.524	1.00	10.86
ATOM	2284	NZ	LYS	338	6.052	10.123	2.334	1.00	10.86
ATOM	2285	C	LYS	338	10.488	14.372	5.225	1.00	3.30
ATOM	2286	O	LYS	338	10.169	15.553	5.329	1.00	10.86
ATOM	2287	N	MET	339	11.242	13.752	6.123	1.00	2.00
ATOM	2288	CA	MET	339	11.725	14.425	7.316	1.00	2.00
ATOM	2289	CB	MET	339	12.139	13.396	8.375	1.00	2.00
ATOM	2290	CG	MET	339	10.999	12.536	8.901	1.00	2.00
ATOM	2291	SD	MET	339	11.504	11.362	10.161	1.00	2.00
ATOM	2292	CE	MET	339	10.004	11.147	10.942	1.00	2.00
ATOM	2293	C	MET	339	12.868	15.396	7.064	1.00	2.00
ATOM	2294	O	MET	339	12.906	16.483	7.638	1.00	2.00
ATOM	2295	N	LEU	340	13.806	15.012	6.213	1.00	2.00
ATOM	2296	CA	LEU	340	14.915	15.894	5.930	1.00	2.00
ATOM	2297	CB	LEU	340	16.172	15.110	5.603	1.00	7.41

FIG. 3NN

ATOM	2298	CG	LEU	340	16.789	14.652	6.915	1.00	7.41
ATOM	2299	CD1	LEU	340	18.085	13.954	6.639	1.00	7.41
ATOM	2300	CD2	LEU	340	17.013	15.839	7.837	1.00	7.41
ATOM	2301	C	LEU	340	14.600	16.919	4.867	1.00	2.00
ATOM	2302	O	LEU	340	15.307	17.051	3.882	1.00	7.41
ATOM	2303	N	VAL	341	13.535	17.668	5.111	1.00	12.82
ATOM	2304	CA	VAL	341	13.080	18.721	4.226	1.00	12.82
ATOM	2305	CB	VAL	341	11.574	18.576	3.963	1.00	9.51
ATOM	2306	CG1	VAL	341	11.089	19.709	3.100	1.00	9.51
ATOM	2307	CG2	VAL	341	11.294	17.253	3.300	1.00	9.51
ATOM	2308	C	VAL	341	13.383	20.063	4.914	1.00	12.82
ATOM	2309	O	VAL	341	13.079	20.238	6.093	1.00	9.51
ATOM	2310	N	ILE	342	14.000	20.996	4.190	1.00	4.21
ATOM	2311	CA	ILE	342	14.364	22.298	4.748	1.00	4.21
ATOM	2312	CB	ILE	342	15.462	22.984	3.900	1.00	6.31
ATOM	2313	CG2	ILE	342	15.799	24.360	4.452	1.00	6.31
ATOM	2314	CG1	ILE	342	16.719	22.108	3.900	1.00	6.31
ATOM	2315	CD1	ILE	342	17.843	22.656	3.067	1.00	6.31
ATOM	2316	C	ILE	342	13.182	23.224	4.975	1.00	4.21
ATOM	2317	O	ILE	342	13.117	23.883	6.016	1.00	6.31
ATOM	2318	N	ASP	343	12.236	23.255	4.041	1.00	2.00
ATOM	2319	CA	ASP	343	11.065	24.108	4.191	1.00	2.00
ATOM	2320	CB	ASP	343	10.494	24.501	2.823	1.00	21.74
ATOM	2321	CG	ASP	343	9.258	25.414	2.926	1.00	21.74
ATOM	2322	OD1	ASP	343	9.113	26.183	3.915	1.00	21.74
ATOM	2323	OD2	ASP	343	8.421	25.366	1.998	1.00	21.74
ATOM	2324	C	ASP	343	10.009	23.390	5.026	1.00	2.00
ATOM	2325	O	ASP	343	9.532	22.328	4.654	1.00	21.74
ATOM	2326	N	PRO	344	9.661	23.949	6.191	1.00	12.51
ATOM	2327	CD	PRO	344	10.281	25.161	6.751	1.00	16.37
ATOM	2328	CA	PRO	344	8.660	23.408	7.120	1.00	12.51
ATOM	2329	CB	PRO	344	8.633	24.449	8.234	1.00	16.37
ATOM	2330	CG	PRO	344	9.997	25.012	8.214	1.00	16.37
ATOM	2331	C	PRO	344	7.269	23.236	6.516	1.00	12.51
ATOM	2332	O	PRO	344	6.469	22.473	7.040	1.00	16.37
ATOM	2333	N	ALA	345	6.960	23.979	5.455	1.00	11.95
ATOM	2334	CA	ALA	345	5.657	23.872	4.816	1.00	11.95
ATOM	2335	CB	ALA	345	5.416	25.044	3.881	1.00	9.14
ATOM	2336	C	ALA	345	5.515	22.558	4.070	1.00	11.95
ATOM	2337	O	ALA	345	4.420	22.018	3.967	1.00	9.14
ATOM	2338	N	LYS	346	6.634	22.036	3.580	1.00	2.00
ATOM	2339	CA	LYS	346	6.655	20.776	2.840	1.00	2.00
ATOM	2340	CB	LYS	346	7.534	20.923	1.595	1.00	15.05
ATOM	2341	CG	LYS	346	6.984	21.930	0.601	1.00	15.05
ATOM	2342	CD	LYS	346	8.067	22.442	-0.340	1.00	15.05
ATOM	2343	CE	LYS	346	7.529	23.576	-1.222	1.00	15.05
ATOM	2344	NZ	LYS	346	7.093	24.764	-0.427	1.00	15.05
ATOM	2345	C	LYS	346	7.131	19.597	3.695	1.00	2.00
ATOM	2346	O	LYS	346	7.046	18.442	3.279	1.00	15.05
ATOM	2347	N	ARG	347	7.602	19.900	4.903	1.00	2.00
ATOM	2348	CA	ARG	347	8.081	18.881	5.828	1.00	2.00
ATOM	2349	CB	ARG	347	8.913	19.498	6.939	1.00	3.45
ATOM	2350	CG	ARG	347	9.801	18.490	7.598	1.00	3.45
ATOM	2351	CD	ARG	347	10.512	19.071	8.775	1.00	3.45
ATOM	2352	NE	ARG	347	11.486	20.074	8.377	1.00	3.45
ATOM	2353	CZ	ARG	347	11.548	21.294	8.893	1.00	3.45
ATOM	2354	NH1	ARG	347	10.686	21.662	9.833	1.00	3.45
ATOM	2355	NH2	ARG	347	12.452	22.157	8.450	1.00	3.45
ATOM	2356	C	ARG	347	6.906	18.134	6.431	1.00	2.00

FIG. 300

ATOM	2357	O	ARG	347	5.832	18.694	6.614	1.00	3.45
ATOM	2358	N	ILE	348	7.120	16.860	6.732	1.00	2.29
ATOM	2359	CA	ILE	348	6.088	15.991	7.288	1.00	2.29
ATOM	2360	CB	ILE	348	6.431	14.489	7.057	1.00	2.00
ATOM	2361	CG2	ILE	348	7.530	14.026	8.012	1.00	2.00
ATOM	2362	CG1	ILE	348	5.174	13.639	7.234	1.00	2.00
ATOM	2363	CD1	ILE	348	5.351	12.213	6.784	1.00	2.00
ATOM	2364	C	ILE	348	5.821	16.240	8.758	1.00	2.29
ATOM	2365	O	ILE	348	6.733	16.518	9.532	1.00	2.00
ATOM	2366	N	SER	349	4.550	16.127	9.127	1.00	5.28
ATOM	2367	CA	SER	349	4.106	16.351	10.494	1.00	5.28
ATOM	2368	CB	SER	349	2.612	16.722	10.515	1.00	14.72
ATOM	2369	OG	SER	349	1.814	15.800	9.786	1.00	14.72
ATOM	2370	C	SER	349	4.357	15.122	11.350	1.00	5.28
ATOM	2371	O	SER	349	4.721	14.067	10.839	1.00	14.72
ATOM	2372	N	VAL	350	4.146	15.251	12.653	1.00	20.79
ATOM	2373	CA	VAL	350	4.357	14.140	13.561	1.00	20.79
ATOM	2374	CB	VAL	350	4.321	14.594	15.044	1.00	18.92
ATOM	2375	CG1	VAL	350	4.677	13.434	15.953	1.00	18.92
ATOM	2376	CG2	VAL	350	5.296	15.740	15.269	1.00	18.92
ATOM	2377	C	VAL	350	3.296	13.071	13.325	1.00	20.79
ATOM	2378	O	VAL	350	3.606	11.883	13.340	1.00	18.92
ATOM	2379	N	ASP	351	2.063	13.495	13.055	1.00	2.00
ATOM	2380	CA	ASP	351	0.953	12.568	12.827	1.00	2.00
ATOM	2381	CB	ASP	351	-0.371	13.321	12.900	1.00	23.45
ATOM	2382	CG	ASP	351	-0.559	14.012	14.234	1.00	23.45
ATOM	2383	OD1	ASP	351	-0.281	15.234	14.320	1.00	23.45
ATOM	2384	OD2	ASP	351	-0.945	13.316	15.198	1.00	23.45
ATOM	2385	C	ASP	351	1.024	11.760	11.545	1.00	2.00
ATOM	2386	O	ASP	351	0.484	10.661	11.468	1.00	23.45
ATOM	2387	N	ASP	352	1.674	12.315	10.531	1.00	17.97
ATOM	2388	CA	ASP	352	1.829	11.616	9.263	1.00	17.97
ATOM	2389	CB	ASP	352	1.957	12.598	8.108	1.00	2.54
ATOM	2390	CG	ASP	352	0.642	13.267	7.759	1.00	2.54
ATOM	2391	OD1	ASP	352	-0.436	12.730	8.135	1.00	2.54
ATOM	2392	OD2	ASP	352	0.695	14.329	7.118	1.00	2.54
ATOM	2393	C	ASP	352	3.024	10.699	9.314	1.00	17.97
ATOM	2394	O	ASP	352	3.035	9.667	8.648	1.00	2.54
ATOM	2395	N	ALA	353	4.011	11.064	10.129	1.00	2.00
ATOM	2396	CA	ALA	353	5.224	10.270	10.310	1.00	2.00
ATOM	2397	CB	ALA	353	6.289	11.079	11.024	1.00	13.93
ATOM	2398	C	ALA	353	4.884	9.014	11.107	1.00	2.00
ATOM	2399	O	ALA	353	5.600	8.024	11.044	1.00	13.93
ATOM	2400	N	LEU	354	3.769	9.063	11.831	1.00	2.00
ATOM	2401	CA	LEU	354	3.300	7.942	12.629	1.00	2.00
ATOM	2402	CB	LEU	354	2.517	8.458	13.827	1.00	10.71
ATOM	2403	CG	LEU	354	3.359	9.011	14.967	1.00	10.71
ATOM	2404	CD1	LEU	354	2.548	10.017	15.749	1.00	10.71
ATOM	2405	CD2	LEU	354	3.860	7.875	15.853	1.00	10.71
ATOM	2406	C	LEU	354	2.431	7.001	11.811	1.00	2.00
ATOM	2407	O	LEU	354	2.219	5.854	12.198	1.00	10.71
ATOM	2408	N	GLN	355	1.889	7.517	10.709	1.00	2.00
ATOM	2409	CA	GLN	355	1.049	6.745	9.806	1.00	2.00
ATOM	2410	CB	GLN	355	-0.143	7.571	9.331	1.00	23.61
ATOM	2411	CG	GLN	355	-1.341	7.508	10.258	1.00	23.61
ATOM	2412	CD	GLN	355	-1.835	6.078	10.499	1.00	23.61
ATOM	2413	OE1	GLN	355	-2.113	5.678	11.638	1.00	23.61
ATOM	2414	NE2	GLN	355	-1.951	5.304	9.419	1.00	23.61
ATOM	2415	C	GLN	355	1.854	6.263	8.613	1.00	2.00

FIG. 3PP

ATOM	2416	O	GLN	355	1.308	5.669	7.686	1.00	23.61
ATOM	2417	N	HIS	356	3.157	6.505	8.651	1.00	2.14
ATOM	2418	CA	HIS	356	4.042	6.074	7.584	1.00	2.14
ATOM	2419	CB	HIS	356	5.407	6.747	7.735	1.00	10.92
ATOM	2420	CG	HIS	356	6.262	6.667	6.510	1.00	10.92
ATOM	2421	CD2	HIS	356	7.183	5.756	6.117	1.00	10.92
ATOM	2422	ND1	HIS	356	6.227	7.626	5.523	1.00	10.92
ATOM	2423	CE1	HIS	356	7.094	7.311	4.577	1.00	10.92
ATOM	2424	NE2	HIS	356	7.686	6.180	4.915	1.00	10.92
ATOM	2425	C	HIS	356	4.186	4.553	7.711	1.00	2.14
ATOM	2426	O	HIS	356	4.341	4.040	8.808	1.00	10.92
ATOM	2427	N	PRO	357	4.132	3.818	6.590	1.00	13.41
ATOM	2428	CD	PRO	357	3.937	4.297	5.213	1.00	36.38
ATOM	2429	CA	PRO	357	4.262	2.356	6.619	1.00	13.41
ATOM	2430	CB	PRO	357	4.321	1.981	5.134	1.00	36.38
ATOM	2431	CG	PRO	357	4.691	3.289	4.432	1.00	36.38
ATOM	2432	C	PRO	357	5.476	1.836	7.397	1.00	13.41
ATOM	2433	O	PRO	357	5.395	0.788	8.043	1.00	36.38
ATOM	2434	N	TYR	358	6.590	2.563	7.371	1.00	5.90
ATOM	2435	CA	TYR	358	7.765	2.113	8.098	1.00	5.90
ATOM	2436	CB	TYR	358	8.996	2.933	7.709	1.00	6.75
ATOM	2437	CG	TYR	358	10.315	2.361	8.174	1.00	6.75
ATOM	2438	CD1	TYR	358	10.694	1.069	7.851	1.00	6.75
ATOM	2439	CE1	TYR	358	11.943	0.571	8.214	1.00	6.75
ATOM	2440	CD2	TYR	358	11.218	3.143	8.877	1.00	6.75
ATOM	2441	CE2	TYR	358	12.465	2.653	9.245	1.00	6.75
ATOM	2442	CZ	TYR	358	12.826	1.369	8.905	1.00	6.75
ATOM	2443	OH	TYR	358	14.074	0.902	9.247	1.00	6.75
ATOM	2444	C	TYR	358	7.503	2.210	9.604	1.00	5.90
ATOM	2445	O	TYR	358	8.002	1.385	10.356	1.00	6.75
ATOM	2446	N	ILE	359	6.672	3.169	10.030	1.00	20.57
ATOM	2447	CA	ILE	359	6.357	3.387	11.457	1.00	20.57
ATOM	2448	CB	ILE	359	6.402	4.917	11.829	1.00	2.00
ATOM	2449	CG2	ILE	359	6.153	5.121	13.318	1.00	2.00
ATOM	2450	CG1	ILE	359	7.754	5.527	11.478	1.00	2.00
ATOM	2451	CD1	ILE	359	8.870	5.038	12.334	1.00	2.00
ATOM	2452	C	ILE	359	5.022	2.835	11.996	1.00	20.57
ATOM	2453	O	ILE	359	4.980	2.229	13.070	1.00	2.00
ATOM	2454	N	ASN	360	3.943	3.040	11.249	1.00	11.50
ATOM	2455	CA	ASN	360	2.600	2.617	11.647	1.00	11.50
ATOM	2456	CB	ASN	360	1.587	2.863	10.519	1.00	15.91
ATOM	2457	CG	ASN	360	1.535	1.720	9.513	1.00	15.91
ATOM	2458	OD1	ASN	360	2.554	1.310	8.974	1.00	15.91
ATOM	2459	ND2	ASN	360	0.338	1.198	9.270	1.00	15.91
ATOM	2460	C	ASN	360	2.490	1.170	12.110	1.00	11.50
ATOM	2461	O	ASN	360	1.581	0.836	12.871	1.00	15.91
ATOM	2462	N	VAL	361	3.415	0.318	11.670	1.00	2.00
ATOM	2463	CA	VAL	361	3.374	-1.083	12.050	1.00	2.00
ATOM	2464	CB	VAL	361	4.517	-1.914	11.398	1.00	43.19
ATOM	2465	CG1	VAL	361	4.397	-1.886	9.872	1.00	43.19
ATOM	2466	CG2	VAL	361	5.885	-1.429	11.860	1.00	43.19
ATOM	2467	C	VAL	361	3.400	-1.280	13.565	1.00	2.00
ATOM	2468	O	VAL	361	3.067	-2.357	14.051	1.00	43.19
ATOM	2469	N	TRP	362	3.742	-0.234	14.311	1.00	2.00
ATOM	2470	CA	TRP	362	3.794	-0.325	15.766	1.00	2.00
ATOM	2471	CB	TRP	362	5.143	0.178	16.285	1.00	4.01
ATOM	2472	CG	TRP	362	6.316	-0.475	15.704	1.00	4.01
ATOM	2473	CD2	TRP	362	6.938	-1.674	16.168	1.00	4.01
ATOM	2474	CE2	TRP	362	8.076	-1.890	15.371	1.00	4.01

FIG. 3QQ

ATOM	2475	CE3	TRP	362	6.643	-2.580	17.189	1.00	4.01
ATOM	2476	CD1	TRP	362	7.074	-0.028	14.666	1.00	4.01
ATOM	2477	NE1	TRP	362	8.135	-0.872	14.459	1.00	4.01
ATOM	2478	CZ2	TRP	362	8.928	-2.987	15.566	1.00	4.01
ATOM	2479	CZ3	TRP	362	7.482	-3.662	17.383	1.00	4.01
ATOM	2480	CH2	TRP	362	8.614	-3.857	16.578	1.00	4.01
ATOM	2481	C	TRP	362	2.716	0.497	16.454	1.00	2.00
ATOM	2482	O	TRP	362	2.496	0.329	17.641	1.00	4.01
ATOM	2483	N	TYR	363	2.039	1.362	15.706	1.00	9.42
ATOM	2484	CA	TYR	363	1.013	2.268	16.228	1.00	9.42
ATOM	2485	CB	TYR	363	0.181	2.843	15.073	1.00	9.22
ATOM	2486	CG	TYR	363	-0.775	3.962	15.439	1.00	9.22
ATOM	2487	CD1	TYR	363	-2.064	3.688	15.899	1.00	9.22
ATOM	2488	CE1	TYR	363	-2.966	4.716	16.182	1.00	9.22
ATOM	2489	CD2	TYR	363	-0.409	5.296	15.278	1.00	9.22
ATOM	2490	CE2	TYR	363	-1.300	6.331	15.568	1.00	9.22
ATOM	2491	CZ	TYR	363	-2.577	6.031	16.016	1.00	9.22
ATOM	2492	OH	TYR	363	-3.485	7.023	16.296	1.00	9.22
ATOM	2493	C	TYR	363	0.091	1.694	17.301	1.00	9.42
ATOM	2494	O	TYR	363	-0.451	0.590	17.150	1.00	9.22
ATOM	2495	N	ASP	364	-0.073	2.461	18.381	1.00	23.57
ATOM	2496	CA	ASP	364	-0.923	2.100	19.516	1.00	23.57
ATOM	2497	CB	ASP	364	-0.078	1.494	20.651	1.00	8.62
ATOM	2498	CG	ASP	364	-0.916	0.800	21.737	1.00	8.62
ATOM	2499	OD1	ASP	364	-2.053	1.246	22.034	1.00	8.62
ATOM	2500	OD2	ASP	364	-0.420	-0.191	22.309	1.00	8.62
ATOM	2501	C	ASP	364	-1.579	3.399	19.971	1.00	23.57
ATOM	2502	O	ASP	364	-0.894	4.376	20.268	1.00	8.62
ATOM	2503	N	PRO	365	-2.918	3.433	20.004	1.00	26.34
ATOM	2504	CD	PRO	365	-3.819	2.313	19.698	1.00	36.54
ATOM	2505	CA	PRO	365	-3.676	4.616	20.429	1.00	26.34
ATOM	2506	CB	PRO	365	-5.117	4.102	20.455	1.00	36.54
ATOM	2507	CG	PRO	365	-5.117	3.016	19.417	1.00	36.54
ATOM	2508	C	PRO	365	-3.252	5.043	21.824	1.00	26.34
ATOM	2509	O	PRO	365	-3.057	6.224	22.099	1.00	36.54
ATOM	2510	N	ALA	366	-3.084	4.049	22.691	1.00	34.81
ATOM	2511	CA	ALA	366	-2.691	4.273	24.067	1.00	34.81
ATOM	2512	CB	ALA	366	-2.627	2.952	24.811	1.00	23.80
ATOM	2513	C	ALA	366	-1.357	4.979	24.143	1.00	34.81
ATOM	2514	O	ALA	366	-1.198	5.915	24.924	1.00	23.80
ATOM	2515	N	GLU	367	-0.418	4.577	23.292	1.00	15.56
ATOM	2516	CA	GLU	367	0.911	5.181	23.301	1.00	15.56
ATOM	2517	CB	GLU	367	1.942	4.223	22.707	1.00	54.26
ATOM	2518	CG	GLU	367	2.018	2.895	23.446	1.00	54.26
ATOM	2519	CD	GLU	367	2.873	1.832	22.736	1.00	54.26
ATOM	2520	OE1	GLU	367	3.056	1.883	21.492	1.00	54.26
ATOM	2521	OE2	GLU	367	3.357	0.914	23.431	1.00	54.26
ATOM	2522	C	GLU	367	0.941	6.489	22.549	1.00	15.56
ATOM	2523	O	GLU	367	1.694	7.393	22.897	1.00	54.26
ATOM	2524	N	VAL	368	0.080	6.610	21.550	1.00	52.58
ATOM	2525	CA	VAL	368	0.056	7.812	20.736	1.00	52.58
ATOM	2526	CB	VAL	368	-0.258	7.459	19.252	1.00	22.16
ATOM	2527	CG1	VAL	368	-0.404	8.721	18.421	1.00	22.16
ATOM	2528	CG2	VAL	368	0.850	6.585	18.680	1.00	22.16
ATOM	2529	C	VAL	368	-0.931	8.863	21.239	1.00	52.58
ATOM	2530	O	VAL	368	-0.549	9.931	21.738	1.00	22.16
ATOM	2531	N	GLU	369	-2.206	8.533	21.097	1.00	23.43
ATOM	2532	CA	GLU	369	-3.300	9.396	21.484	1.00	23.43
ATOM	2533	CB	GLU	369	-4.561	8.988	20.707	1.00	53.35

FIG. 3RR

ATOM	2534	CG	GLU	369	-4.450	9.125	19.182	1.00	53.35
ATOM	2535	CD	GLU	369	-4.518	10.581	18.692	1.00	53.35
ATOM	2536	OE1	GLU	369	-4.879	11.498	19.474	1.00	53.35
ATOM	2537	OE2	GLU	369	-4.208	10.816	17.503	1.00	53.35
ATOM	2538	C	GLU	369	-3.566	9.381	22.987	1.00	23.43
ATOM	2539	O	GLU	369	-4.699	9.155	23.424	1.00	53.35
ATOM	2540	N	ALA	370	-2.516	9.615	23.770	1.00	27.26
ATOM	2541	CA	ALA	370	-2.618	9.660	25.228	1.00	27.26
ATOM	2542	CB	ALA	370	-1.253	9.371	25.858	1.00	10.16
ATOM	2543	C	ALA	370	-3.123	11.050	25.640	1.00	27.26
ATOM	2544	O	ALA	370	-2.923	12.021	24.912	1.00	10.16
ATOM	2545	N	PRO	371	-3.773	11.159	26.824	1.00	34.01
ATOM	2546	CD	PRO	371	-3.949	10.062	27.792	1.00	40.77
ATOM	2547	CA	PRO	371	-4.325	12.420	27.362	1.00	34.01
ATOM	2548	CB	PRO	371	-5.076	11.950	28.619	1.00	40.77
ATOM	2549	CG	PRO	371	-4.226	10.810	29.103	1.00	40.77
ATOM	2550	C	PRO	371	-3.266	13.483	27.699	1.00	34.01
ATOM	2551	O	PRO	371	-2.400	13.277	28.559	1.00	40.77
ATOM	2552	N	PRO	372	-3.331	14.638	27.011	1.00	14.63
ATOM	2553	CD	PRO	372	-4.378	14.947	26.018	1.00	28.09
ATOM	2554	CA	PRO	372	-2.420	15.770	27.183	1.00	14.63
ATOM	2555	CB	PRO	372	-2.940	16.769	26.143	1.00	28.09
ATOM	2556	CG	PRO	372	-4.418	16.447	26.055	1.00	28.09
ATOM	2557	C	PRO	372	-2.499	16.334	28.598	1.00	14.63
ATOM	2558	O	PRO	372	-3.589	16.532	29.141	1.00	28.09
ATOM	2559	N	PRO	373	-1.335	16.504	29.245	1.00	51.40
ATOM	2560	CD	PRO	373	-0.041	16.052	28.704	1.00	51.87
ATOM	2561	CA	PRO	373	-1.181	17.035	30.609	1.00	51.40
ATOM	2562	CB	PRO	373	0.241	16.601	30.982	1.00	51.87
ATOM	2563	CG	PRO	373	0.963	16.653	29.668	1.00	51.87
ATOM	2564	C	PRO	373	-1.353	18.567	30.635	1.00	51.40
ATOM	2565	O	PRO	373	-0.819	19.271	29.765	1.00	51.87
ATOM	2566	N	ALA	374	-2.120	19.071	31.613	1.00	42.06
ATOM	2567	CA	ALA	374	-2.381	20.507	31.726	1.00	42.06
ATOM	2568	CB	ALA	374	-3.811	20.734	32.250	1.00	31.44
ATOM	2569	C	ALA	374	-1.350	21.373	32.499	1.00	42.06
ATOM	2570	O	ALA	374	-1.519	22.592	32.621	1.00	31.44
ATOM	2571	N	ALA	375	-0.290	20.751	33.010	1.00	38.52
ATOM	2572	CA	ALA	375	0.761	21.480	33.735	1.00	38.52
ATOM	2573	CB	ALA	375	1.602	22.327	32.752	1.00	29.54
ATOM	2574	C	ALA	375	0.182	22.364	34.848	1.00	38.52
ATOM	2575	O	ALA	375	0.312	23.594	34.798	1.00	29.54
ATOM	2576	N	TYR	376	-0.385	21.710	35.874	1.00	47.67
ATOM	2577	CA	TYR	376	-1.024	22.369	37.024	1.00	47.67
ATOM	2578	CB	TYR	376	-0.030	23.174	37.857	1.00	78.81
ATOM	2579	CG	TYR	376	-0.681	23.843	39.065	1.00	78.81
ATOM	2580	CD1	TYR	376	-0.993	23.100	40.207	1.00	78.81
ATOM	2581	CE1	TYR	376	-1.555	23.703	41.345	1.00	78.81
ATOM	2582	CD2	TYR	376	-0.954	25.218	39.085	1.00	78.81
ATOM	2583	CE2	TYR	376	-1.520	25.834	40.228	1.00	78.81
ATOM	2584	CZ	TYR	376	-1.813	25.064	41.350	1.00	78.81
ATOM	2585	OH	TYR	376	-2.336	25.628	42.493	1.00	78.81
ATOM	2586	C	TYR	376	-2.129	23.307	36.564	1.00	47.67
ATOM	2587	O	TYR	376	-3.319	23.018	36.729	1.00	78.81
ATOM	2588	N	ALA	377	-1.714	24.451	36.029	1.00	45.97
ATOM	2589	CA	ALA	377	-2.621	25.459	35.526	1.00	45.97
ATOM	2590	CB	ALA	377	-2.819	26.547	36.574	1.00	46.05
ATOM	2591	C	ALA	377	-1.996	26.034	34.252	1.00	45.97
ATOM	2592	O	ALA	377	-2.274	25.555	33.138	1.00	46.05

FIG. 3SS

ATOM	2593	N	ALA	378	-1.112	27.019	34.430	1.00	45.78
ATOM	2594	CA	ALA	378	-0.422	27.673	33.312	1.00	45.78
ATOM	2595	CB	ALA	378	-1.391	28.607	32.545	1.00	26.15
ATOM	2596	C	ALA	378	0.814	28.450	33.785	1.00	45.78
ATOM	2597	O	ALA	378	1.016	29.599	33.400	1.00	26.15
ATOM	2598	N	ALA	379	1.645	27.807	34.607	1.00	29.23
ATOM	2599	CA	ALA	379	2.866	28.434	35.106	1.00	29.23
ATOM	2600	CB	ALA	379	3.634	27.463	36.003	1.00	29.46
ATOM	2601	C	ALA	379	3.730	28.822	33.902	1.00	29.23
ATOM	2602	O	ALA	379	4.216	27.940	33.183	1.00	29.46
ATOM	2603	N	LEU	380	3.862	30.128	33.644	1.00	45.66
ATOM	2604	CA	LEU	380	4.681	30.608	32.522	1.00	45.66
ATOM	2605	CB	LEU	380	4.506	32.117	32.319	1.00	31.66
ATOM	2606	CG	LEU	380	3.081	32.622	32.111	1.00	31.66
ATOM	2607	CD1	LEU	380	3.140	33.905	31.285	1.00	31.66
ATOM	2608	CD2	LEU	380	2.240	31.568	31.385	1.00	31.66
ATOM	2609	C	LEU	380	6.167	30.299	32.691	1.00	45.66
ATOM	2610	O	LEU	380	6.924	31.141	33.173	1.00	31.66
ATOM	2611	N	ASP	381	6.586	29.114	32.248	1.00	30.99
ATOM	2612	CA	ASP	381	7.983	28.706	32.378	1.00	30.99
ATOM	2613	CB	ASP	381	8.162	27.266	31.901	1.00	18.50
ATOM	2614	CG	ASP	381	7.219	26.300	32.596	1.00	18.50
ATOM	2615	OD1	ASP	381	6.254	25.858	31.935	1.00	18.50
ATOM	2616	OD2	ASP	381	7.442	25.975	33.785	1.00	18.50
ATOM	2617	C	ASP	381	8.982	29.639	31.678	1.00	30.99
ATOM	2618	O	ASP	381	10.175	29.642	32.019	1.00	18.50
ATOM	2619	N	ALA	382	8.505	30.385	30.676	1.00	60.09
ATOM	2620	CA	ALA	382	9.324	31.366	29.951	1.00	60.09
ATOM	2621	CB	ALA	382	8.879	31.475	28.520	1.00	18.75
ATOM	2622	C	ALA	382	9.055	32.684	30.706	1.00	60.09
ATOM	2623	O	ALA	382	8.280	33.536	30.250	1.00	18.75
ATOM	2624	N	ARG	383	9.678	32.803	31.883	1.00	31.28
ATOM	2625	CA	ARG	383	9.516	33.940	32.794	1.00	31.28
ATOM	2626	CB	ARG	383	8.867	33.415	34.072	1.00	38.51
ATOM	2627	CG	ARG	383	9.491	32.070	34.526	1.00	38.51
ATOM	2628	CD	ARG	383	8.900	31.514	35.807	1.00	38.51
ATOM	2629	NE	ARG	383	7.524	31.050	35.649	1.00	38.51
ATOM	2630	CZ	ARG	383	6.556	31.266	36.536	1.00	38.51
ATOM	2631	NH1	ARG	383	6.808	31.946	37.653	1.00	38.51
ATOM	2632	NH2	ARG	383	5.334	30.791	36.321	1.00	38.51
ATOM	2633	C	ARG	383	10.873	34.547	33.143	1.00	31.28
ATOM	2634	O	ARG	383	11.902	33.911	32.932	1.00	38.51
ATOM	2635	N	ALA	384	10.885	35.765	33.687	1.00	38.58
ATOM	2636	CA	ALA	384	12.148	36.409	34.067	1.00	38.58
ATOM	2637	CB	ALA	384	12.397	37.634	33.209	1.00	22.57
ATOM	2638	C	ALA	384	12.268	36.762	35.555	1.00	38.58
ATOM	2639	O	ALA	384	11.458	37.519	36.107	1.00	22.57
ATOM	2640	N	HIS	385	13.297	36.211	36.195	1.00	13.25
ATOM	2641	CA	HIS	385	13.545	36.434	37.618	1.00	13.25
ATOM	2642	CB	HIS	385	13.005	35.283	38.447	1.00	5.73
ATOM	2643	CG	HIS	385	11.537	35.076	38.326	1.00	5.73
ATOM	2644	CD2	HIS	385	10.803	34.416	37.402	1.00	5.73
ATOM	2645	ND1	HIS	385	10.651	35.516	39.281	1.00	5.73
ATOM	2646	CE1	HIS	385	9.430	35.126	38.958	1.00	5.73
ATOM	2647	NE2	HIS	385	9.496	34.456	37.820	1.00	5.73
ATOM	2648	C	HIS	385	15.024	36.533	37.906	1.00	13.25
ATOM	2649	O	HIS	385	15.859	36.234	37.065	1.00	5.73
ATOM	2650	N	THR	386	15.351	36.946	39.114	1.00	13.73
ATOM	2651	CA	THR	386	16.744	37.043	39.494	1.00	13.73

FIG. 3TT

ATOM	2652	CB	THR	386	17.000	38.204	40.462	1.00	34.39
ATOM	2653	OG1	THR	386	15.920	38.298	41.406	1.00	34.39
ATOM	2654	CG2	THR	386	17.157	39.506	39.699	1.00	34.39
ATOM	2655	C	THR	386	17.138	35.762	40.185	1.00	13.73
ATOM	2656	O	THR	386	16.287	34.920	40.469	1.00	34.39
ATOM	2657	N	ILE	387	18.433	35.641	40.469	1.00	7.70
ATOM	2658	CA	ILE	387	19.008	34.499	41.162	1.00	7.70
ATOM	2659	CB	ILE	387	20.492	34.743	41.442	1.00	16.33
ATOM	2660	CG2	ILE	387	21.076	33.621	42.300	1.00	16.33
ATOM	2661	CG1	ILE	387	21.255	34.893	40.126	1.00	16.33
ATOM	2662	CD1	ILE	387	22.736	35.136	40.334	1.00	16.33
ATOM	2663	C	ILE	387	18.286	34.300	42.491	1.00	7.70
ATOM	2664	O	ILE	387	17.898	33.188	42.815	1.00	16.33
ATOM	2665	N	ALA	388	18.098	35.379	43.247	1.00	2.00
ATOM	2666	CA	ALA	388	17.404	35.299	44.521	1.00	2.00
ATOM	2667	CB	ALA	388	17.384	36.658	45.183	1.00	28.05
ATOM	2668	C	ALA	388	15.984	34.762	44.363	1.00	2.00
ATOM	2669	O	ALA	388	15.559	33.901	45.128	1.00	28.05
ATOM	2670	N	GLU	389	15.264	35.246	43.353	1.00	18.37
ATOM	2671	CA	GLU	389	13.880	34.818	43.095	1.00	18.37
ATOM	2672	CB	GLU	389	13.183	35.797	42.161	1.00	30.68
ATOM	2673	CG	GLU	389	13.070	37.191	42.725	1.00	30.68
ATOM	2674	CD	GLU	389	12.680	38.226	41.684	1.00	30.68
ATOM	2675	OE1	GLU	389	12.475	37.877	40.503	1.00	30.68
ATOM	2676	OE2	GLU	389	12.583	39.408	42.051	1.00	30.68
ATOM	2677	C	GLU	389	13.800	33.431	42.483	1.00	18.37
ATOM	2678	O	GLU	389	12.827	32.704	42.706	1.00	30.68
ATOM	2679	N	TRP	390	14.803	33.086	41.684	1.00	13.76
ATOM	2680	CA	TRP	390	14.858	31.786	41.044	1.00	13.76
ATOM	2681	CB	TRP	390	15.978	31.743	40.006	1.00	7.41
ATOM	2682	CG	TRP	390	15.576	32.219	38.639	1.00	7.41
ATOM	2683	CD2	TRP	390	14.552	31.663	37.790	1.00	7.41
ATOM	2684	CE2	TRP	390	14.564	32.401	36.591	1.00	7.41
ATOM	2685	CE3	TRP	390	13.619	30.632	37.935	1.00	7.41
ATOM	2686	CD1	TRP	390	16.149	33.229	37.932	1.00	7.41
ATOM	2687	NE1	TRP	390	15.554	33.341	36.701	1.00	7.41
ATOM	2688	CZ2	TRP	390	13.692	32.121	35.530	1.00	7.41
ATOM	2689	CZ3	TRP	390	12.750	30.358	36.883	1.00	7.41
ATOM	2690	CH2	TRP	390	12.789	31.104	35.700	1.00	7.41
ATOM	2691	C	TRP	390	15.116	30.733	42.110	1.00	13.76
ATOM	2692	O	TRP	390	14.447	29.707	42.144	1.00	7.41
ATOM	2693	N	LYS	391	16.074	31.011	42.987	1.00	3.15
ATOM	2694	CA	LYS	391	16.415	30.116	44.076	1.00	3.15
ATOM	2695	CB	LYS	391	17.491	30.768	44.945	1.00	17.74
ATOM	2696	CG	LYS	391	17.794	30.047	46.246	1.00	17.74
ATOM	2697	CD	LYS	391	19.069	30.592	46.886	1.00	17.74
ATOM	2698	CE	LYS	391	19.494	29.775	48.113	1.00	17.74
ATOM	2699	NZ	LYS	391	20.841	30.179	48.640	1.00	17.74
ATOM	2700	C	LYS	391	15.140	29.861	44.881	1.00	3.15
ATOM	2701	O	LYS	391	14.837	28.719	45.242	1.00	17.74
ATOM	2702	N	GLU	392	14.372	30.920	45.119	1.00	2.00
ATOM	2703	CA	GLU	392	13.126	30.814	45.859	1.00	2.00
ATOM	2704	CB	GLU	392	12.483	32.190	45.996	1.00	47.37
ATOM	2705	CG	GLU	392	11.075	32.162	46.601	1.00	47.37
ATOM	2706	CD	GLU	392	11.088	32.382	48.104	1.00	47.37
ATOM	2707	OE1	GLU	392	11.463	33.502	48.526	1.00	47.37
ATOM	2708	OE2	GLU	392	10.726	31.447	48.860	1.00	47.37
ATOM	2709	C	GLU	392	12.151	29.896	45.141	1.00	2.00
ATOM	2710	O	GLU	392	11.522	29.027	45.757	1.00	47.37

FIG. 3UU

ATOM	2711	N	LEU	393	12.018	30.118	43.835	1.00	3.75
ATOM	2712	CA	LEU	393	11.114	29.356	42.990	1.00	3.75
ATOM	2713	CB	LEU	393	11.083	29.958	41.594	1.00	2.00
ATOM	2714	CG	LEU	393	10.159	31.146	41.373	1.00	2.00
ATOM	2715	CD1	LEU	393	10.352	31.661	39.962	1.00	2.00
ATOM	2716	CD2	LEU	393	8.727	30.707	41.598	1.00	2.00
ATOM	2717	C	LEU	393	11.487	27.894	42.882	1.00	3.75
ATOM	2718	O	LEU	393	10.620	27.029	42.840	1.00	2.00
ATOM	2719	N	ILE	394	12.787	27.632	42.857	1.00	11.25
ATOM	2720	CA	ILE	394	13.343	26.291	42.734	1.00	11.25
ATOM	2721	CB	ILE	394	14.839	26.396	42.406	1.00	2.00
ATOM	2722	CG2	ILE	394	15.516	25.028	42.423	1.00	2.00
ATOM	2723	CG1	ILE	394	14.969	27.090	41.050	1.00	2.00
ATOM	2724	CD1	ILE	394	16.345	27.169	40.524	1.00	2.00
ATOM	2725	C	ILE	394	13.104	25.456	43.980	1.00	11.25
ATOM	2726	O	ILE	394	12.649	24.313	43.901	1.00	2.00
ATOM	2727	N	TYR	395	13.391	26.058	45.127	1.00	24.41
ATOM	2728	CA	TYR	395	13.194	25.437	46.422	1.00	24.41
ATOM	2729	CB	TYR	395	13.752	26.378	47.492	1.00	24.18
ATOM	2730	CG	TYR	395	13.750	25.851	48.903	1.00	24.18
ATOM	2731	CD1	TYR	395	14.749	24.997	49.355	1.00	24.18
ATOM	2732	CE1	TYR	395	14.784	24.574	50.685	1.00	24.18
ATOM	2733	CD2	TYR	395	12.787	26.267	49.810	1.00	24.18
ATOM	2734	CE2	TYR	395	12.816	25.854	51.138	1.00	24.18
ATOM	2735	CZ	TYR	395	13.811	25.013	51.570	1.00	24.18
ATOM	2736	OH	TYR	395	13.823	24.643	52.892	1.00	24.18
ATOM	2737	C	TYR	395	11.696	25.153	46.638	1.00	24.41
ATOM	2738	O	TYR	395	11.329	24.060	47.040	1.00	24.18
ATOM	2739	N	LYS	396	10.824	26.100	46.312	1.00	7.12
ATOM	2740	CA	LYS	396	9.387	25.887	46.486	1.00	7.12
ATOM	2741	CB	LYS	396	8.596	27.142	46.099	1.00	14.43
ATOM	2742	CG	LYS	396	8.648	28.257	47.134	1.00	14.43
ATOM	2743	CD	LYS	396	7.966	29.513	46.634	1.00	14.43
ATOM	2744	CE	LYS	396	7.873	30.571	47.723	1.00	14.43
ATOM	2745	NZ	LYS	396	7.321	31.859	47.188	1.00	14.43
ATOM	2746	C	LYS	396	8.851	24.689	45.711	1.00	7.12
ATOM	2747	O	LYS	396	7.824	24.118	46.082	1.00	14.43
ATOM	2748	N	GLU	397	9.549	24.318	44.640	1.00	27.91
ATOM	2749	CA	GLU	397	9.146	23.197	43.790	1.00	27.91
ATOM	2750	CB	GLU	397	9.576	23.428	42.330	1.00	25.61
ATOM	2751	CG	GLU	397	9.153	22.327	41.339	1.00	25.61
ATOM	2752	CD	GLU	397	7.720	22.464	40.856	1.00	25.61
ATOM	2753	OE1	GLU	397	7.134	23.535	41.111	1.00	25.61
ATOM	2754	OE2	GLU	397	7.183	21.526	40.213	1.00	25.61
ATOM	2755	C	GLU	397	9.752	21.901	44.309	1.00	27.91
ATOM	2756	O	GLU	397	9.094	20.855	44.301	1.00	25.61
ATOM	2757	N	VAL	398	11.003	21.976	44.761	1.00	19.14
ATOM	2758	CA	VAL	398	11.701	20.813	45.296	1.00	19.14
ATOM	2759	CB	VAL	398	13.206	21.106	45.592	1.00	2.00
ATOM	2760	CG1	VAL	398	13.939	19.825	45.941	1.00	2.00
ATOM	2761	CG2	VAL	398	13.857	21.769	44.402	1.00	2.00
ATOM	2762	C	VAL	398	11.016	20.382	46.594	1.00	19.14
ATOM	2763	O	VAL	398	10.810	19.185	46.829	1.00	2.00
ATOM	2764	N	MET	399	10.642	21.366	47.420	1.00	22.42
ATOM	2765	CA	MET	399	9.969	21.114	48.693	1.00	22.42
ATOM	2766	CB	MET	399	10.111	22.305	49.635	1.00	20.89
ATOM	2767	CG	MET	399	10.947	21.968	50.854	1.00	20.89
ATOM	2768	SD	MET	399	12.603	21.419	50.367	1.00	20.89
ATOM	2769	CE	MET	399	13.360	21.155	52.002	1.00	20.89

FIG. 3VV

ATOM	2770	C	MET	399	8.504	20.808	48.455	1.00	22.42
ATOM	2771	O	MET	399	7.891	20.052	49.210	1.00	20.89
ATOM	2772	N	ASN	400	7.948	21.403	47.406	1.00	28.60
ATOM	2773	CA	ASN	400	6.565	21.150	47.049	1.00	28.60
ATOM	2774	CB	ASN	400	6.481	19.736	46.459	1.00	81.18
ATOM	2775	CG	ASN	400	5.100	19.387	45.951	1.00	81.18
ATOM	2776	OD1	ASN	400	4.599	18.282	46.199	1.00	81.18
ATOM	2777	ND2	ASN	400	4.479	20.318	45.219	1.00	81.18
ATOM	2778	C	ASN	400	5.629	21.282	48.257	1.00	28.60
ATOM	2779	O	ASN	400	5.257	22.426	48.589	1.00	81.18
ATOM	2780	C5	3400	1001	22.736	4.627	31.172	1.00	20.00
ATOM	2781	C2	3400	1001	22.276	5.904	31.111	1.00	20.00
ATOM	2782	N1	3400	1001	23.156	6.818	30.322	1.00	20.00
ATOM	2783	C4	3400	1001	24.235	6.108	29.848	1.00	20.00
ATOM	2784	S1	3400	1001	24.123	4.375	30.081	1.00	20.00
ATOM	2785	C15	3400	1001	27.483	6.454	27.874	1.00	20.00
ATOM	2786	N3	3400	1001	27.589	7.776	27.927	1.00	20.00
ATOM	2787	C17	3400	1001	26.749	8.622	28.538	1.00	20.00
ATOM	2788	C11	3400	1001	25.618	8.113	29.190	1.00	20.00
ATOM	2789	C13	3400	1001	25.444	6.726	29.175	1.00	20.00
ATOM	2790	C19	3400	1001	26.367	5.887	28.516	1.00	20.00
ATOM	2791	C1	3400	1001	20.021	10.016	32.442	1.00	20.00
ATOM	2792	C9	3400	1001	19.766	8.582	32.361	1.00	20.00
ATOM	2793	C3	3400	1001	18.521	8.129	32.868	1.00	20.00
ATOM	2794	C12	3400	1001	17.569	9.048	33.425	1.00	20.00
ATOM	2795	C20	3400	1001	17.887	10.433	33.471	1.00	20.00
ATOM	2796	C6	3400	1001	19.111	11.000	32.997	1.00	20.00
ATOM	2797	C7	3400	1001	20.961	6.391	31.694	1.00	20.00
ATOM	2798	O3	3400	1001	20.137	5.549	32.029	1.00	20.00
ATOM	2799	N2	3400	1001	20.762	7.730	31.764	1.00	20.00
ATOM	2800	C8	3400	1001	19.395	12.627	33.166	1.00	20.00
ATOM	2801	F3	3400	1001	20.299	13.330	32.210	1.00	20.00
ATOM	2802	F2	3400	1001	20.027	12.609	34.486	1.00	20.00
ATOM	2803	F1	3400	1001	18.169	13.443	33.069	1.00	20.00

END

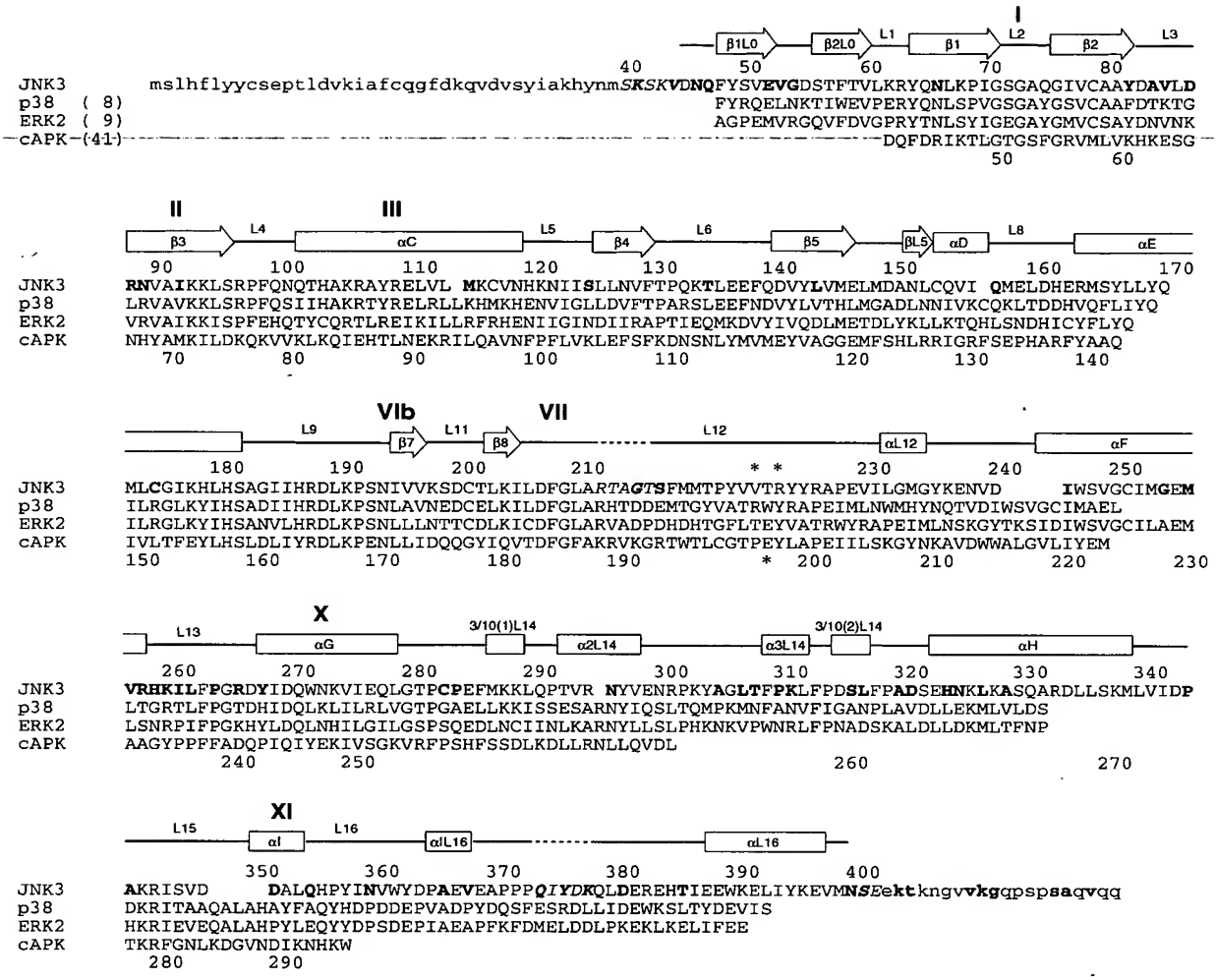
I
β1L0
β2L0
L1
β1
L2
β2
L3
JNK3 mslhflyycseptldvkiafcqgfdkqvdvsyiakhynmSKSKVDNQFYSVEVGDSTFTVLKRYQNLKPIGSGAQGIVCAAYDAVLD
p38 (8) FYRQELNKTIWEVPERYQNLSPVGSGAYGSVCAAFDTKTG
ERK2 (9) AGPEMVRGQVFDVGPRYTNLSYIGEGAYGMVCSAYDNVNK
cAPK (41) DQFDRIKTLGTGSFGRVMLVKHKESG
II
III
β3
L4
αC
L5
β4
L6
β5
βL5
αD
L8
αE
JNK3 RNVAIKKLSRPFQNQTHAKRAYRELVL MKCVNHKNIISLLNVFTPQKTLEEFQDVYLVMELMDANLCQVI QMELDHERMSYLLYQ
p38 LRVAVKKLSRPFQSIIHAKRTYRELRLLKHMKHENVIGLLDVFTPARSLEEFNDVYLVTHLMGADLNNIVKCQKLTDDHVQFLIYQ
ERK2 VRVAIKKISPFEHQTYCQRTLREIKILLRFRHENIIGINDIIRAPTIEQMKDVYIVQDLMETDLYKLLKTQHLSNDHICYFLYQ
cAPK NHYAMKILDKQKVVKLKQIEHTLNEKRILQAVNFPFLVKLEFSFKDNSNLYMVMEYVAGGEMFSHLRRIGRFSEPHARFYAAQ
VIb
VII
L9
β7
L11
β8
L12
αL12
αF
JNK3 MLCGIKHLHSAGIIHRDLKPSNIVVKSDCTLKILDFGLARTAGTSFMMTPYVVTRYYRAPEVILGMGYKENVD IWSVGCIMGEM
p38 ILRGLKYIHSADIIHRDLKPSNLAVNEDCELKILDFGLARHTDDEMTGYVATRWYRAPEIMLNWMHYNQTVDIWSVGCIMAEL
ERK2 ILRGLKYIHSANVLHRDLKPSNLLLNTTCDLKICDFGLARVADPDHDHTGFLTEYVATRWYRAPEIMLNSKGYTKSIDIWSVGCILAEM
cAPK IVLTFEYLHSLDLIYRDLKPENLLIDQQGYIQVTDFGFAKRVKGRTWTLCGTPEYLAPEIILSKGYNKAVDWWALGVLIYEM
X
L13
αG
3/10(1)L14
α2L14
3/10(2)L14
α3L14
αH
JNK3 VRHKILFPGRDYIDQWNKVIEQLGTPCPEFMKKLQPTVR NYVENRPKYAGLTFPKLFPDSLFPADSEHNKLKASQARDLLSKMLVIDP
p38 LTGRTLFPGTDHIDQLKLILRLVGTPGAELLKKISSESARNYIQSLTQMPKMNFANVFIGANPLAVDLLEKMLVLDS
ERK2 LSNRPIFPGKHYLDQLNHILGILGSPSQEDLNCIINLKARNYLLSLPHKNKVPWNRLFPNADSKALDLLDKMLTFNP
cAPK AAGYPPFFADQPIQIYEKIVSGKVRFPSHFSSDLKDLLRNLLQVDL
XI
L15
αI
L16
αIL16
αL16
JNK3 AKRISVD DALQHPYINVWYDPAEVEAPPPQIYDKQLDEREHTIEEWKELIYKEVMNSEektkngvvkgqpspsaqvqq
p38 DKRITAAQALAHAYFAQYHDPDDEPVADPYDQSFESRDLLIDEWKSLTYDEVIS
ERK2 HKRIEVEQALAHPYLEQYYDPSDEPIAEAPFKFDMELDDLPKEKLKELIFEE
cAPK TKRFGNLKDGVNDIKNHKW

FIG. 4

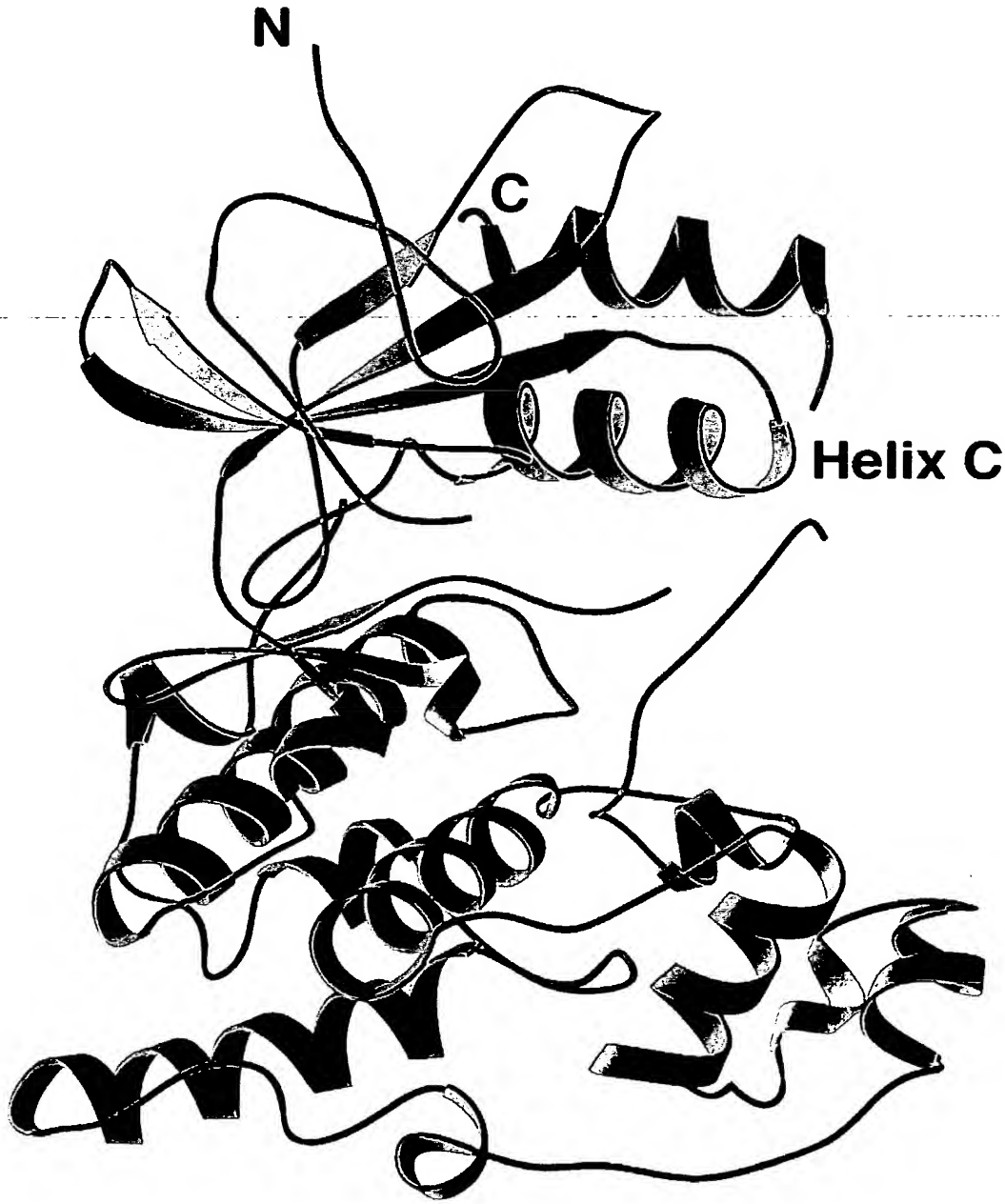

FIG. 5

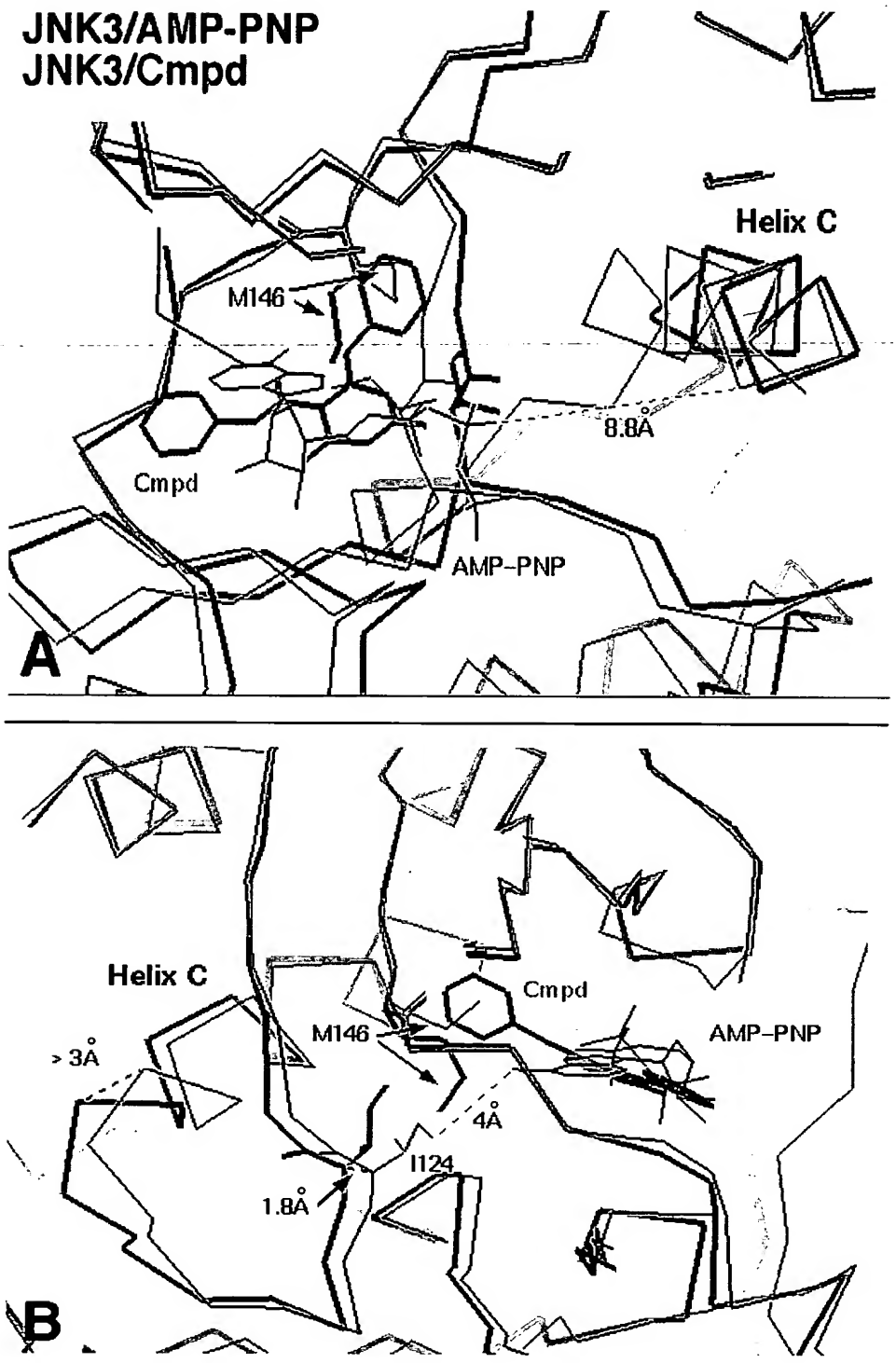
JNK3/AMP-PNP
JNK3/Cmpd
Helix C
M146
8.8Å
Cmpd
AMP-PNP
A
Helix C
Cmpd
M146
AMP-PNP
> 3Å
4Å
I124
1.8Å
B

FIG. 6

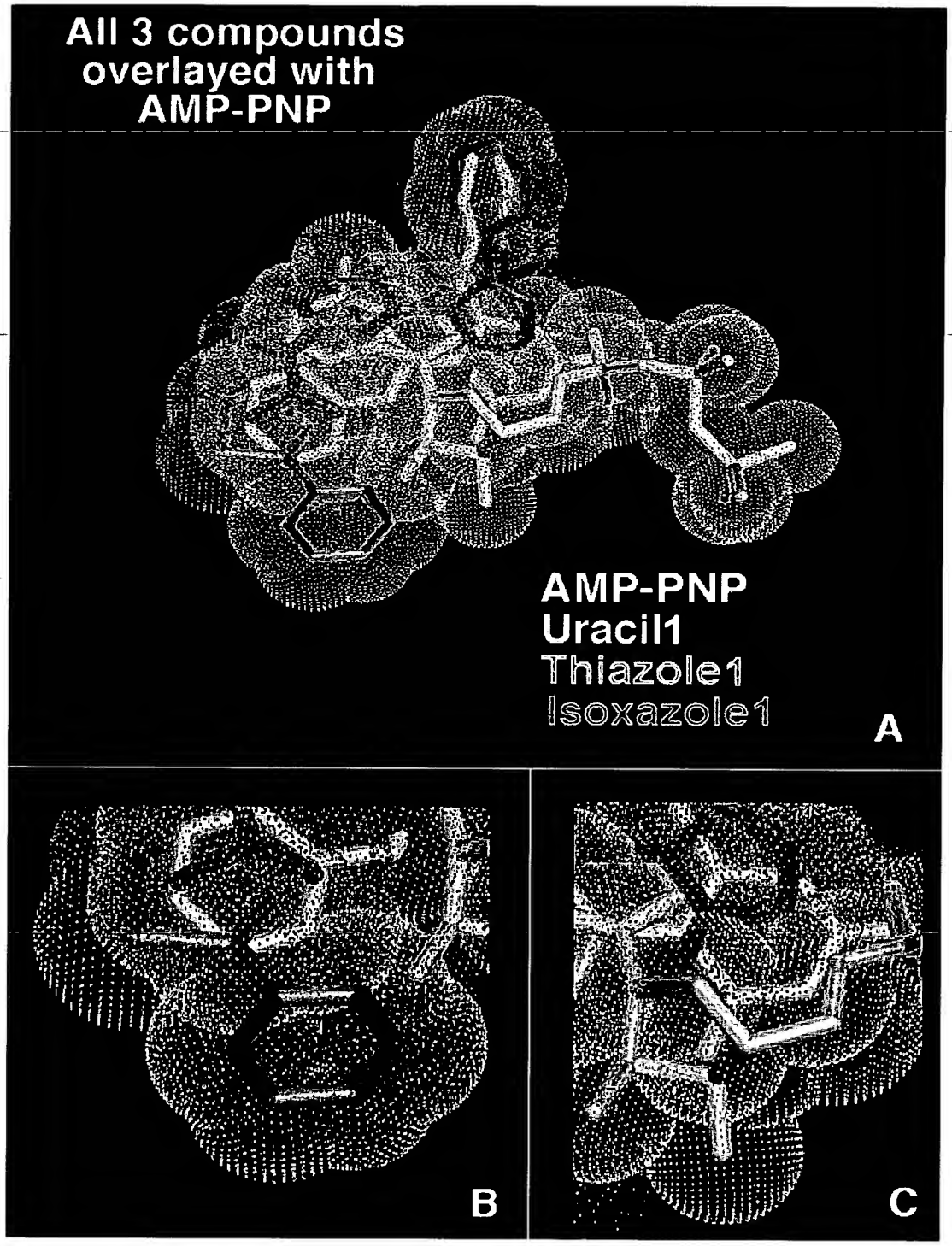

FIG. 7

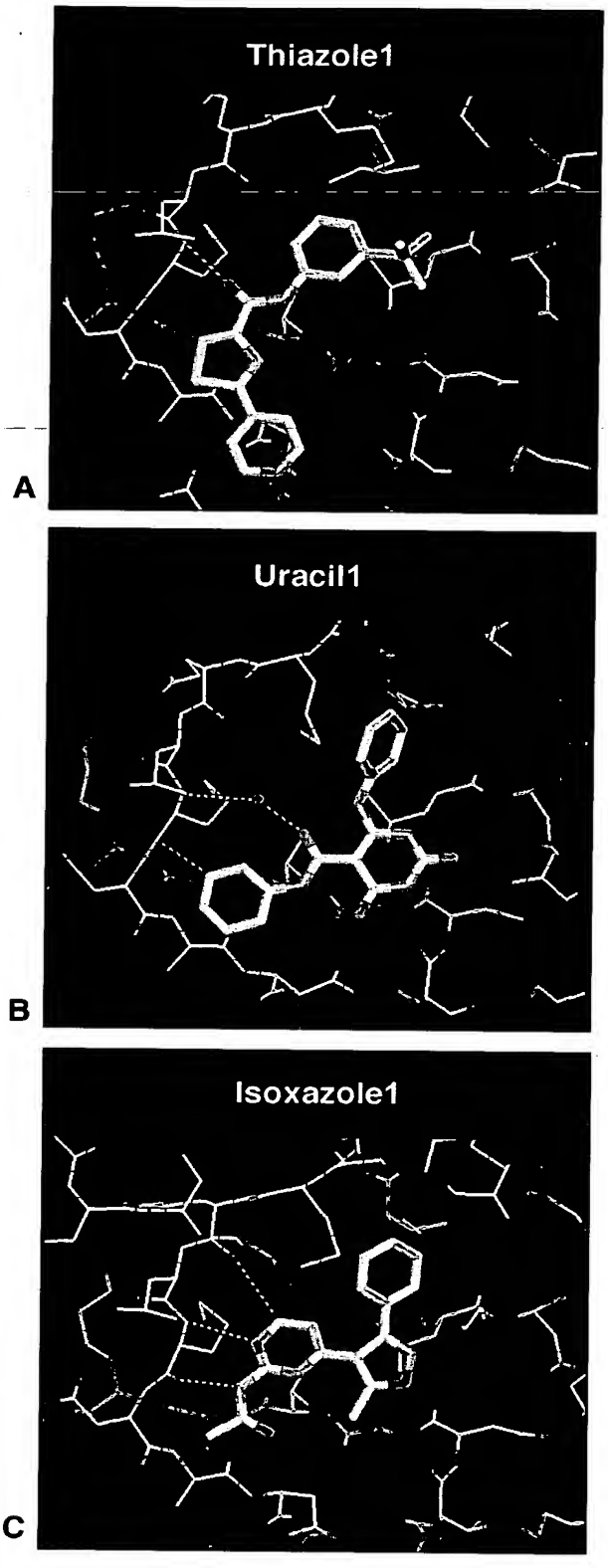

FIG. 8

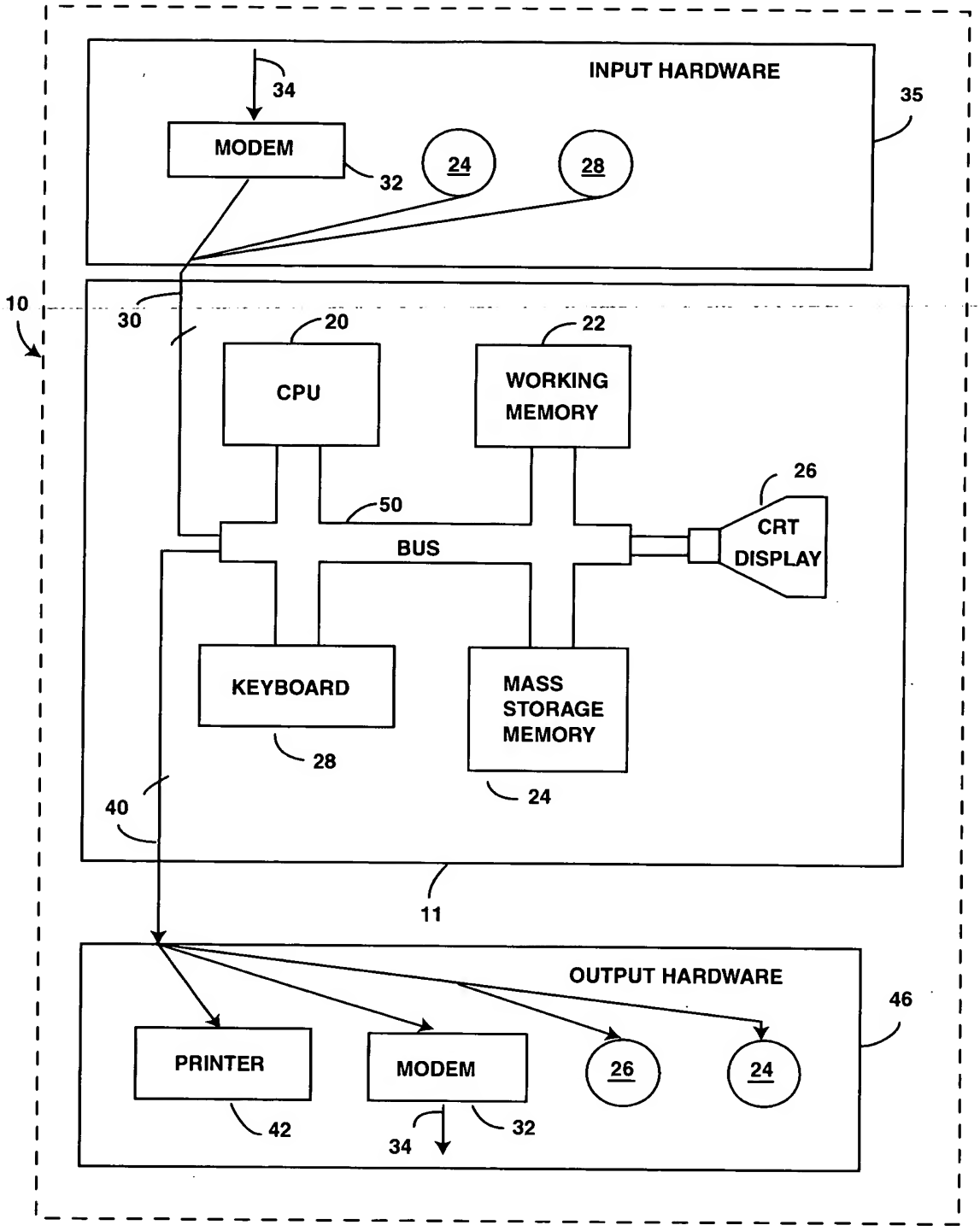
INPUT HARDWARE
34
35
MODEM
32
24
28
10
30
20
22
CPU
WORKING MEMORY
26
50
BUS
CRT DISPLAY
KEYBOARD
MASS STORAGE MEMORY
28
24
40
11
OUTPUT HARDWARE
46
PRINTER
MODEM
26
24
42
34
32

FIG. 9

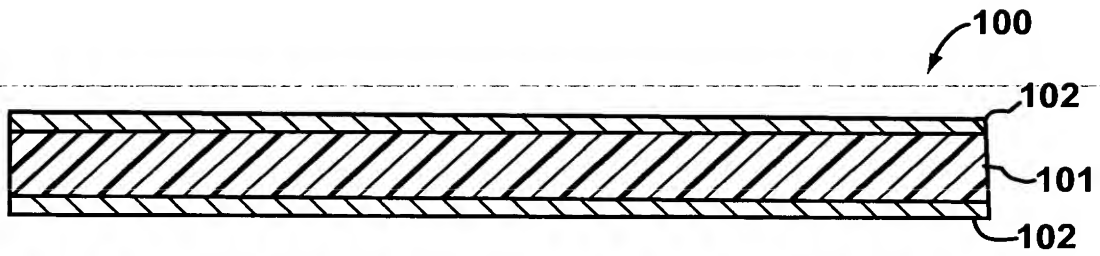

FIG. 10

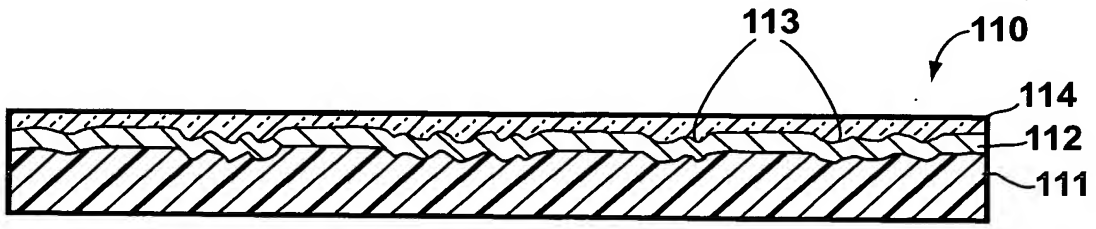

FIG. 11